



SM358

Additional Exercises for Book 2

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This set of exercises relates to Book 2 of SM358 and can be used for further practice and for revision purposes. To gain maximum benefit, it is important to attempt each question for yourself before looking up the solution.

Exercises

Topic 1 — Dirac notation

Exercise 1.1 Given that $|c\rangle = |a\rangle + i|b\rangle$ where $|a\rangle$ and $|b\rangle$ are vectors that are normalized but not necessarily orthogonal, show that

$$\langle c|c\rangle = 2(1 - \text{Im}(\langle a|b\rangle)).$$

Exercise 1.2 If $|a\rangle$ and $|b\rangle$ are any non-zero ket vectors, and

$$|c\rangle = |a\rangle - \frac{\langle b|a\rangle}{\langle b|b\rangle} |b\rangle,$$

show that $|c\rangle$ is orthogonal to $|b\rangle$.

In the special case $|b\rangle = \lambda|a\rangle$, where λ is any non-zero complex constant, show that $|c\rangle$ is the zero vector.

Exercise 1.3 Suppose that A and B are observables with discrete non-degenerate eigenvalues in a given system. Suppose that $|\alpha_i\rangle$ is a state in which A is certain to have the value a_i , and $|\beta_j\rangle$ is a state in which B is certain to have the value b_j . Show that the probability of obtaining the result b_j when B is measured in the state $|\alpha_i\rangle$ is the same as the probability of obtaining the result a_i when A is measured in the state $|\beta_j\rangle$.

Exercise 1.4 Write out explicitly the meaning of $\langle \phi | \hat{O} | \psi \rangle$ in each of the following cases:

- (a) $|\phi\rangle$ and $|\psi\rangle$ are represented by functions $\phi(x)$ and $\psi(x)$ of the coordinate x , and $\hat{O} = d^2/dx^2$.
- (b) $|\phi\rangle$ and $|\psi\rangle$ are represented by functions $\phi(x, y, z)$ and $\psi(x, y, z)$ of the Cartesian coordinates x, y and z , and $\hat{O} = \partial^2/\partial x^2$.
- (c) $|\phi\rangle, |\psi\rangle$ and \hat{O} are represented by the matrices:

$$|\phi\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}, \quad |\psi\rangle = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad \text{and} \quad \hat{O} = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix}.$$

Topic 2 — Hermitian operators

Exercise 2.1 Define what is meant by a Hermitian operator. By integrating both sides of the identity

$$\frac{d}{dx} \left(\psi^*(x) \frac{d\phi}{dx} - \frac{d\psi^*}{dx} \phi(x) \right) = \psi^*(x) \frac{d^2\phi}{dx^2} - \frac{d^2\psi^*}{dx^2} \phi(x),$$

show that d^2/dx^2 is a Hermitian operator.

Exercise 2.2 Show that, if \hat{A} and \hat{B} are Hermitian operators, then

$$\hat{C} = \hat{A} \hat{B} \hat{A}$$

is also a Hermitian operator.

Exercise 2.3 If \hat{A} and \hat{B} are Hermitian operators, show that

$$\langle \phi | \hat{A} \hat{B} | \psi \rangle = \langle \psi | \hat{B} \hat{A} | \phi \rangle^*,$$

where $|\phi\rangle$ and $|\psi\rangle$ are normalizable vectors.

Exercise 2.4 In this question \hat{A} is a Hermitian operator with a discrete set of eigenvalues a_n and corresponding eigenvectors $|\phi_n\rangle$:

$$\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle.$$

The vector $|\psi\rangle$ is a linear combination of eigenvectors of \hat{A} corresponding to different eigenvalues:

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle,$$

where the c_n are complex coefficients.

Use the above information to show mathematically that

$$\langle \psi | \hat{A} | \psi \rangle = \sum_n |c_n|^2 a_n.$$

Point out explicitly where the Hermitian nature of \hat{A} has been used in your derivation.

Exercise 2.5 Show that, if \hat{A} is a Hermitian operator, then the expectation value of the corresponding observable A is real in any state Ψ .

Topic 3 — Commutators and generalized Ehrenfest theorem

Exercise 3.1 Suppose that an observable A is represented by an operator \hat{A} that commutes with the Hamiltonian operator \hat{H} of a system. Show that, for any state of this system, the expectation value $\langle A \rangle$ and the square of the uncertainty, $(\Delta A)^2$, are independent of time.

Exercise 3.2 (a) If \hat{H} is the Hamiltonian operator for a system and $|\psi_n\rangle$ is an eigenvector of \hat{H} with eigenvalue E_n , show that

$$\langle \psi_n | [\hat{A}, \hat{H}] | \psi_n \rangle = 0$$

for any operator \hat{A} . You will need to use the fact that \hat{H} is a Hermitian operator.

(b) Use your answer to part (a) to show that $d\langle A \rangle / dt = 0$ in any energy eigenstate.

Exercise 3.3 A particle of mass m is described by the Hamiltonian operator

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \frac{1}{2}C(x^2 + y^2)$$

where C is a constant.

Use the generalized Ehrenfest theorem to show that $\langle p_z \rangle$ remains constant in time in this system.

Exercise 3.4 By allowing the commutator to act on an arbitrary function, or otherwise, show that

$$[\hat{p}_x, \hat{x}^2] = -2i\hbar\hat{x}.$$

Hence express the rate of change of $\langle p_x \rangle$ in terms of $\langle x \rangle$ for a particle subject to the harmonic oscillator potential energy function $V(x) = \frac{1}{2}Cx^2$.

Exercise 3.5 By allowing the commutator to act on an arbitrary function, or otherwise, show that

$$[\hat{x}, \hat{p}_x^2] = 2i\hbar\hat{p}_x.$$

Hence use the generalized Ehrenfest theorem to show that

$$\frac{d\langle x \rangle}{dt} = \frac{\langle p_x \rangle}{m}$$

for a particle of mass m .

Exercise 3.6 (a) By allowing the commutator to act on an arbitrary function, show that

$$[\hat{p}_x, V(x)] = -i\hbar \frac{dV}{dx}.$$

(b) By expanding the commutators, show that

$$\hat{p}_x [\hat{p}_x, V(x)] + [\hat{p}_x, V(x)] \hat{p}_x = [\hat{p}_x^2, V(x)].$$

Hence use the result of part (a) to show that

$$[\hat{p}_x^2, V(x)] = -i\hbar \left(\hat{p}_x \frac{dV}{dx} + \frac{dV}{dx} \hat{p}_x \right).$$

Exercise 3.7 For a one-dimensional system with Hamiltonian operator

$$\hat{H} = \hat{E}_{\text{kin}} + \hat{V} = \frac{\hat{p}_x^2}{2m} + V(x),$$

use the generalized Ehrenfest theorem and the result of Exercise 3.6(b) to show that

$$\frac{d\langle E_{\text{kin}} \rangle}{dt} = -\frac{1}{2m} \left\langle \hat{p}_x \frac{dV}{dx} + \frac{dV}{dx} \hat{p}_x \right\rangle.$$

Apply this result to find the rate of change of the expectation value of the kinetic energy in the special case $V(x) = mgx$.

Topic 4 — Orbital angular momentum

Exercise 4.1 Given that $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$, use the generalized uncertainty principle to show that, if a system is in a state with a definite non-zero value of L_z , it cannot have a definite value of either L_x or L_y .

Exercise 4.2 When the Stern–Gerlach experiment is carried out with silver atoms, two distinct traces are produced on a detecting screen. Explain why this implies the quantization of angular momentum, but cannot be understood if the silver atoms have only orbital angular momentum, with the usual restrictions on quantum numbers.

Exercise 4.3 A particle of mass m is described by the Hamiltonian operator

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + V(x, y, z)$$

where

$$V(x, y, z) = C_1(x^2 + y^2) + C_2z^2$$

and C_1 and C_2 are constants.

Use spherical coordinates to show that \hat{L}_z commutes with $V(x, y, z)$. Hence, given the fact that \hat{L}_z commutes with $\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2$, use the generalized Ehrenfest theorem to show that $\langle L_z \rangle$ remains constant in time in this system.

Exercise 4.4 Suppose that $L_x^2 + L_y^2$ is measured in a state $|l, m\rangle$ with definite values of the orbital angular momentum quantum number, l , and the magnetic quantum number, m . What value will be obtained with certainty? Express your answer in terms of l and m .

Exercise 4.5 Use the Hermitian nature of \hat{L}_z to show that, in any state ψ_m with a definite value of the magnetic quantum number, m ,

$$\langle \psi_m | \hat{L}_y \hat{L}_z | \psi_m \rangle = \langle \psi_m | \hat{L}_z \hat{L}_y | \psi_m \rangle.$$

Hence use the commutation relations for orbital angular momentum to show that $\langle L_x \rangle = 0$ in the state ψ_m .

Exercise 4.6 In any state $|l, m\rangle$ with definite values of the orbital angular momentum quantum number, l , and the magnetic quantum number, m , it can be shown that

$$\langle L_x^2 \rangle = \langle L_y^2 \rangle.$$

Taking this result on trust, and using the results of Exercises 4.4 and 4.5, derive expressions for the uncertainties ΔL_x , ΔL_y and ΔL_z in the state $|l, m\rangle$, and show that these uncertainties are consistent with the generalized uncertainty principle.

Topic 5 — Spin angular momentum

Exercise 5.1 Are the spin states $|\uparrow_x\rangle$ and $|\uparrow_y\rangle$ orthogonal? Explain your answer.

Exercise 5.2 Suppose that a spin- $\frac{1}{2}$ particle is prepared in a state that is spin-up in the x -direction. Use inner products to find the probability that a measurement of its spin component in the \mathbf{n} -direction, corresponding to the spherical coordinates $\theta = 2\pi/3$ and $\phi = \pi/2$, will give spin-up.

You may use the result

$$|\uparrow_{\mathbf{n}}\rangle = \cos(\theta/2)|\uparrow_z\rangle + e^{i\phi} \sin(\theta/2)|\downarrow_z\rangle.$$

Exercise 5.3 (a) Given that

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad |\downarrow_x\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}, \quad |\downarrow_y\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 1 \end{bmatrix}$$

$$|\uparrow_z\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\downarrow_z\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

express the spin state

$$|D\rangle = \frac{1}{5} \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

as a linear combination of:

- (i) the eigenvectors of \hat{S}_x ,
- (ii) the eigenvectors of \hat{S}_y ,
- (iii) the eigenvectors of \hat{S}_z .

(b) What are the probabilities of obtaining spin-up in the x -, y - and z -directions in the spin state $|D\rangle$?

Exercise 5.4 The spin state of a spin- $\frac{1}{2}$ particle is described by the spinor

$$|A\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2i \end{bmatrix}.$$

Find the expectation values of S_x , S_y and S_z in this state. You may use the operators

$$\hat{S}_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{S}_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \text{and} \quad \hat{S}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Exercise 5.5 The spin state of a spin- $\frac{1}{2}$ particle is described by the normalized spinor

$$|A\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix},$$

where $|a_1|^2 + |a_2|^2 = 1$. Express $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$ in terms of a_1 and a_2 and hence show that

$$\langle S_x \rangle^2 + \langle S_y \rangle^2 + \langle S_z \rangle^2 = \frac{\hbar^2}{4}.$$

Exercise 5.6 The general spin state for spin-up in the direction \mathbf{n} is

$$|\uparrow_{\mathbf{n}}\rangle = \cos(\theta/2)|\uparrow_z\rangle + e^{i\phi} \sin(\theta/2)|\downarrow_z\rangle,$$

where θ and ϕ are the spherical coordinates associated with the direction \mathbf{n} . Show that, in this state

$$\langle S_x \rangle = \frac{\hbar}{2} \sin \theta \cos \phi, \quad \langle S_y \rangle = \frac{\hbar}{2} \sin \theta \sin \phi \quad \text{and} \quad \langle S_z \rangle = \frac{\hbar}{2} \cos \theta,$$

which means that the vector $(\langle S_x \rangle, \langle S_y \rangle, \langle S_z \rangle) = (\hbar/2)\mathbf{n}$.

Exercise 5.7 A spin- $\frac{1}{2}$ particle with spin gyromagnetic ratio γ_s is in a uniform magnetic field of magnitude B that points in the y -direction. The Hamiltonian matrix for this system is

$$\hat{H} = -\frac{\gamma_s B \hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}.$$

Show that the spin ket

$$|A\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} e^{i\gamma_s B t/2}$$

satisfies Schrödinger's equation for this system.

Exercise 5.8 A spin- $\frac{1}{2}$ particle with spin gyromagnetic ratio $\gamma_s < 0$ is in a uniform magnetic field of magnitude B that points in the \mathbf{n} -direction. The Hamiltonian operator governing the spin state of the particle is

$$\hat{H} = -\gamma_s B \hat{\mathbf{S}}_{\mathbf{n}}.$$

At time $t = 0$, the spin state of the particle is described by the ket

$$|A\rangle_{\text{initial}} = \frac{1}{\sqrt{2}} (|\uparrow_{\mathbf{n}}\rangle + |\downarrow_{\mathbf{n}}\rangle).$$

Write down an expression for the spin ket of the particle at a time $t \geq 0$, expressing your answer in terms of the Larmor frequency,

$$\omega = |\gamma_s|B = -\gamma_s B.$$

Topic 6 — Many-particle systems

Exercise 6.1 A system composed of two spin- $\frac{1}{2}$ particles is in the spin state

$$|A\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2,$$

where $|\uparrow\rangle_i$ is a spin state of particle i corresponding to the value $S_{z,i} = \hbar/2$ for the z -component of particle i .

Show explicitly that $|A\rangle$ is an eigenvector of $\hat{\mathbf{S}} = \hat{\mathbf{S}}_{z,1} + \hat{\mathbf{S}}_{z,2}$, and find the corresponding eigenvalue.

Exercise 6.2 A single particle in a one-dimensional infinite square well with walls at $x = 0$ and $x = L$ has normalized energy eigenfunctions of the form

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & \text{for } 0 \leq x \leq L \\ 0 & \text{elsewhere} \end{cases}$$

for $n = 1, 2, \dots$

This question concerns a system that is composed of two identical non-interacting spin- $\frac{1}{2}$ particles, in such a well. Write down a normalized total wave function (including spatial and spin parts) that describes the ground state of this two-particle system inside the well at time $t = 0$.

Exercise 6.3 Consider a system of two spin- $\frac{1}{2}$ particles. The operator

$$\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 = \hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y} + \hat{S}_{1,z}\hat{S}_{2,z}$$

refers to various components of the spins of these particles, where the subscripts 1 and 2 are labels for the particles. Given that

$$\hat{\mathbf{S}}^2 = \hat{S}_1^2 + 2\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 + \hat{S}_2^2,$$

find the effect of operating on $|\uparrow\uparrow\rangle$ with $\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2$.

Exercise 6.4 Show that the spin ket

$$|S = 1, M_S = 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

is normalized.

Exercise 6.5 (a) Show explicitly that the function

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} (\phi_A(x_1)\phi_B(x_2) - \phi_B(x_1)\phi_A(x_2))$$

is antisymmetric with respect to interchange of particle labels.

(b) Could a system of two identical spinless particles be described by this spatial function?

(c) If a system of two identical spin- $\frac{1}{2}$ particles is in a state described by this spatial function, what is the total spin angular momentum quantum number, S , in this state?

Exercise 6.6 (a) Given that electrons, protons and neutrons are all spin- $\frac{1}{2}$ particles, determine whether each of the following composite particles is a fermion or a boson.

1. A ${}^4\text{He}$ nucleus (2 protons + 2 neutrons)
2. A ${}^4\text{He}$ atom (2 protons + 2 neutrons + 2 electrons)
3. A ${}^3\text{He}$ nucleus (2 protons + 1 neutron)
4. A ${}^3\text{He}$ atom (2 protons + 1 neutron + 2 electrons).

(b) Under what circumstances might a collection of ${}^3\text{He}$ atoms undergo Bose–Einstein condensation?

Topic 7 — Measurement

Exercise 7.1 An isolated system with a discrete set of energy values is initially in the state

$$\Psi(x, t) = \frac{1}{5} \left(3\psi_1(x) e^{-iE_1 t/\hbar} - 4i\psi_2(x) e^{-iE_2 t/\hbar} \right),$$

where $\psi_1(x)$ and $\psi_2(x)$ are energy eigenfunctions with eigenvalues E_1 and E_2 , respectively. A measurement of the energy is made and the value E_2 is obtained.

- (a) What is the state of the system immediately after the energy measurement? What can be said about the result of a second energy measurement conducted immediately after the first?
- (b) What can be said about the result of a second energy measurement if it is conducted after a considerable delay, during which the system remains isolated from external influences?
- (c) Suppose that a position measurement of the particle is made (to within a small resolution) between the first energy measurement and the energy measurement described in part (b). What can be said about the result of the second energy measurement in this case?

Exercise 7.2 A spin- $\frac{1}{2}$ particle is prepared in a spin state with $S_z = +\hbar/2$. Its spin component is measured in the direction \mathbf{n} , defined by the angles $\theta = 60^\circ$ and $\phi = 0$ of spherical coordinates, and the value $-\hbar/2$ is obtained. Immediately afterwards, the spin of the particle is measured in the z -direction. What is the probability that a value $S_z = +\hbar/2$ will be obtained? You may use the $\cos^2(\theta/2)$ rule.

Topic 8 — Entanglement

Exercise 8.1 In the famous experiment of Aspect and his colleagues, two photons were produced in the entangled state

$$|\text{photon pair}\rangle = \frac{1}{\sqrt{2}} (|VV\rangle + |HH\rangle),$$

where V and H refer to vertical and horizontal polarization relative to the z -axis.

What feature of $|\text{photon pair}\rangle$ ensures that it represents an entangled state? What correlations does this state lead to for polarization measurements taken on the two photons relative to the z -axis? Could any classical model produce similar correlations?

Exercise 8.2 An entangled pair of spin- $\frac{1}{2}$ particles is in the spin state

$$|A\rangle = \frac{1}{\sqrt{3}} (|\uparrow_x \uparrow_y\rangle + |\uparrow_y \uparrow_x\rangle).$$

Given that

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \text{and} \quad |\uparrow_y\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix},$$

show that the state $|A\rangle$ is normalized. What is the probability that both particles will be found to be spin-up in the x -direction?

Topic 9 — Polarization states of light

Exercise 9.1 (a) Quantum teleportation and quantum cryptography exploit the following polarization states of light:

$$|V_\theta\rangle = \cos\theta|V\rangle + \sin\theta|H\rangle \quad \text{and}$$

$$|H_\theta\rangle = -\sin\theta|V\rangle + \cos\theta|H\rangle.$$

Show that $|V_\theta\rangle$ and $|H_\theta\rangle$ are an orthonormal pair if $|V\rangle$ and $|H\rangle$ are.

(b) In one sentence say how the above equations differ, with respect to their θ -dependence, from the corresponding relations for spin- $\frac{1}{2}$ particles.

Exercise 9.2 A photon is in the linear polarization state $|A\rangle = a_1|H\rangle + a_2|V\rangle$, where a_1 and a_2 are real numbers with $a_1^2 + a_2^2 = 1$. A measurement of circular polarization is carried out on this photon. Given that the polarization state corresponding to right-handed circular polarization is

$$|R\rangle = -\frac{1}{\sqrt{2}}(|H\rangle + i|V\rangle),$$

calculate the probability that the measurement on state $|A\rangle$ will give the result of right-handed circular polarization.

Exercise 9.3 The photon polarization states for right-handed circular polarization and left-handed circular polarization are

$$|R\rangle = -\frac{1}{\sqrt{2}}(|H\rangle + i|V\rangle) \quad \text{and} \quad |L\rangle = \frac{1}{\sqrt{2}}(|H\rangle - i|V\rangle),$$

respectively, where $|H\rangle$ and $|V\rangle$ are states of vertical and horizontal polarization relative to a fixed z -axis.

The polarization states

$$|V_\theta\rangle = \cos\theta|V\rangle + \sin\theta|H\rangle$$

$$|H_\theta\rangle = -\sin\theta|V\rangle + \cos\theta|H\rangle$$

correspond to vertical and horizontal polarization relative to an axis in the xz -plane, at an angle of θ radians to the z -axis and $(\pi/2 - \theta)$ radians to the x -axis. Show explicitly that

$$|R_\theta\rangle \equiv -\frac{1}{\sqrt{2}}(|H_\theta\rangle + i|V_\theta\rangle) \quad \text{and} \quad |L_\theta\rangle \equiv \frac{1}{\sqrt{2}}(|H_\theta\rangle - i|V_\theta\rangle),$$

represent exactly the same polarization states as $|R\rangle$ and $|L\rangle$.

Exercise 9.4 Two photons travelling in the same direction are in the entangled polarization state

$$|A\rangle = \frac{1}{\sqrt{2}}(|LR\rangle - |RL\rangle).$$

For both these photons, states of right-handed and left-handed circular polarization are given by $|R\rangle$ and $|L\rangle$ as defined in the previous question. Use this information to show that

$$\frac{1}{\sqrt{2}}(|LR\rangle - |RL\rangle) = \frac{i}{\sqrt{2}}(|VH\rangle - |HV\rangle).$$

Hence show that, if observer 1 measures the polarization of photon 1 and observer 2 measures the polarization of photon 2, their results are certain to disagree if they measure circular polarizations (R or L), or if they measure linear polarizations relative to the z -direction (H or V).

Topic 10 — Quantum information

Exercise 10.1 Consider an observable with two possible values in any given basis.

- (a) What does it mean to say that two bases are complementary to one another for measurements of such an observable?
- (b) What is the angle between two complementary bases used to measure linear photon polarization?
- (c) What is the angle between two complementary bases used to measure a spin component of a spin- $\frac{1}{2}$ particle?

Exercise 10.2 Alice and Bob implement the BB84 protocol using linear photon polarization and two complementary bases R and D, which they each choose at random. The following table contains nine of their results. In row (ii), V and H represent vertical and horizontal polarizations relative to Alice's basis; in row (iv), V and H represent vertical and horizontal polarizations relative to Bob's basis.

	case	1	2	3	4	5	6	7	8	9
(i)	Alice's basis	R	D	D	D	R	R	D	R	R
(ii)	Alice's sent photon	V	H	V	V	H	H	V	H	H
(iii)	Bob's basis	D	D	R	D	R	R	R	D	R
(iv)	Bob's result	V	H	H	V	V	H	V	H	V

- (a) Which of the nine cases can be rejected on the grounds that inappropriate bases have been chosen by Alice and Bob?
- (b) Which, if any, of the cases suggest that an eavesdropper might be present?

Exercise 10.3 Using Ekert's protocol, Alice and Bob use a source of entangled photon-pairs in the polarization state

$$\frac{1}{\sqrt{2}}(|VH\rangle - |HV\rangle)$$

to obtain a secure shared cryptographic key. In each photon pair, the photons travel in opposite directions along the y -axis; Alice measures the polarization of one photon and Bob measures the polarization of the other.

In a fixed coordinate system, Alice chooses to measure polarization along one of three directions in the xz -plane (specified by the angles of rotation $\alpha_1 = 0^\circ$, $\alpha_2 = 45^\circ$ and $\alpha_3 = 22.5^\circ$ and the $+z$ -direction towards the $+x$ -direction). In a similar way, Bob chooses to measure polarization along one of three directions specified by the angles $\beta_1 = 22.5^\circ$, $\beta_2 = -22.5^\circ$ and $\beta_3 = 45^\circ$. Thus there are nine different combinations of angle for polarization measurements, as indicated in the table below:

	$\alpha_1 = 0^\circ$	$\alpha_2 = 45^\circ$	$\alpha_3 = 22.5^\circ$
$\beta_1 = 22.5^\circ$			
$\beta_2 = -22.5^\circ$			X
$\beta_3 = 45^\circ$	X		X

Suppose for simplicity that Bob and Alice discard measurements arising from the combinations marked with an X. Describe briefly how they could use the remaining six combinations of angle to (a) ensure that they both possess the same cryptographic key and (b) verify that no eavesdropping has taken place.

You may use the CHSH inequality

$$|\Sigma| \leq 2 \quad \text{with} \quad \Sigma = C(\alpha_1 - \beta_1) + C(\alpha_1 - \beta_2) + C(\alpha_2 - \beta_1) - C(\alpha_2 - \beta_2)$$

where, for the entangled state given in the question

$$C(\alpha_i - \beta_j) = -\cos[2(\alpha_i - \beta_j)].$$

Exercise 10.4 Photon 1 is in the unknown polarization state

$$|P\rangle = \alpha|V\rangle + \beta|H\rangle \equiv \begin{bmatrix} \alpha \\ \beta \end{bmatrix},$$

where α and β are complex constants with $|\alpha|^2 + |\beta|^2 = 1$. The polarization state of this photon is to be teleported to a distant location with the aid of an entangled pair of photons, 2 and 3. Photon 3 travels to the distant location and it is arranged for photon 2 to form an entangled state with photon 1. The polarization state of the three-photon system can then be represented by

$$|\Psi\rangle_{123} = \frac{1}{2}(|\Psi^-\rangle_{12}|A\rangle_3 + |\Psi^+\rangle_{12}|B\rangle_3 + |\Phi^-\rangle_{12}|C\rangle_3 + |\Phi^+\rangle_{12}|D\rangle_3),$$

where $|\Psi^-\rangle$, $|\Psi^+\rangle$, $|\Phi^-\rangle$ and $|\Phi^+\rangle$ are Bell states and

$$|A\rangle = \begin{bmatrix} \alpha \\ -\beta \end{bmatrix}, \quad |B\rangle = \begin{bmatrix} -\alpha \\ \beta \end{bmatrix}, \quad |C\rangle = \begin{bmatrix} \beta \\ \alpha \end{bmatrix} \quad \text{and} \quad |D\rangle = \begin{bmatrix} -\beta \\ -\alpha \end{bmatrix}$$

are single-photon polarization states.

Suppose that a Bell-state measurement on the entangled pair of photons 1 and 2 gives a result corresponding to $|\Psi^+\rangle_{12}$. What procedure must then be adopted to ensure that the polarization state of photon 3 becomes identical to the initial unknown polarization state of photon 1? Explain why this procedure does not violate the no-cloning theorem.

Solutions

Topic 1 — Dirac notation

Solution 1.1 Given that $|c\rangle = |a\rangle + i|b\rangle$, we have $\langle c| = \langle a| - i\langle b|$, so

$$\begin{aligned}\langle c|c\rangle &= (\langle a| - i\langle b|)(|a\rangle + i|b\rangle) \\ &= \langle a|a\rangle + \langle b|b\rangle + i\langle a|b\rangle - i\langle b|a\rangle.\end{aligned}$$

Because $|a\rangle$ and $|b\rangle$ are normalized vectors, $\langle a|a\rangle = \langle b|b\rangle = 1$. Also, it is a general property of Dirac brackets that $\langle b|a\rangle = \langle a|b\rangle^*$, so

$$\begin{aligned}\langle c|c\rangle &= 1 + 1 + i(\langle a|b\rangle - \langle a|b\rangle^*) \\ &= 2(1 - \text{Im}(\langle a|b\rangle)),\end{aligned}$$

where we have used the fact that, for any complex number $z - z^* = 2i\text{Im}(z)$.

Comments (1) Note how the bra vector $\langle c|$ is constructed from the expression for $|c\rangle$; we change all the kets into bras and replace each coefficient by its complex conjugate.

(2) The final answer is a real quantity because $\text{Im}(\langle a|b\rangle)$ is real. This makes good sense because $\langle c|c\rangle$ is the square of the norm of the vector $|c\rangle$, which is always real (and non-negative).

Solution 1.2 Taking the inner product of $|c\rangle$ and $|b\rangle$ gives

$$\langle b|c\rangle = \langle b|a\rangle - \frac{\langle b|a\rangle}{\langle b|b\rangle}\langle b|b\rangle = 0,$$

so $|c\rangle$ and $|b\rangle$ are orthogonal.

If $|b\rangle = \lambda|a\rangle$, we have $\langle b| = \lambda^*\langle a|$ so

$$|c\rangle = |a\rangle - \frac{\lambda^*\langle a|a\rangle}{\lambda^*\lambda\langle a|a\rangle}\lambda|a\rangle = |0\rangle,$$

where we have used the symbol $|0\rangle$ for the zero vector. The symbol 0 may seem a more natural choice, but this could be confused with the number zero, which is not the same as the zero vector.

Comment The formula given in this question gives us a way of constructing two orthogonal vectors ($|b\rangle$ and $|c\rangle$) from two vectors which point in different directions but are not necessarily orthogonal ($|b\rangle$ and $|a\rangle$). In general, the vector $|c\rangle$ is not normalized.

Solution 1.3 The state $|\alpha_i\rangle$, in which A is certain to have the value a_i , is an eigenvector of \hat{A} with eigenvalue a_i . Similarly, the state $|\beta_j\rangle$, in which B is certain to have the value b_j , is an eigenvector of \hat{B} with eigenvalue b_j .

The probability of obtaining the result b_j in the state $|\alpha_i\rangle$ is therefore

$$p_1 = |\langle \beta_j|\alpha_i\rangle|^2 = \langle \beta_j|\alpha_i\rangle^* \langle \beta_j|\alpha_i\rangle = \langle \alpha_i|\beta_j\rangle \langle \beta_j|\alpha_i\rangle.$$

The probability of obtaining the result a_i in the state $|\beta_j\rangle$ is

$$p_2 = |\langle \alpha_i|\beta_j\rangle|^2 = \langle \alpha_i|\beta_j\rangle^* \langle \alpha_i|\beta_j\rangle = \langle \beta_j|\alpha_i\rangle \langle \alpha_i|\beta_j\rangle.$$

Evidently, $p_1 = p_2$.

Comments (1) For example, if a_i has probability 0.5 when b_j is certain, then b_j has probability 0.5 when a_i is certain.

(2) The quantum-mechanical result is underpinned by a geometric fact: if $|\alpha_i\rangle$ and $|\beta_j\rangle$ are normalized vectors, the square of the magnitude of the projection of $|\alpha_i\rangle$ on $|\beta_j\rangle$ is equal to the square of the magnitude of the projection of $|\beta_j\rangle$ on $|\alpha_i\rangle$.

Solution 1.4 (a) When $|\phi\rangle$ and $|\psi\rangle$ are represented by $\phi(x)$ and $\psi(x)$, and $\hat{O} = d^2/dx^2$, we have

$$\langle \phi | \hat{O} | \psi \rangle = \int_{-\infty}^{\infty} \phi^*(x) \frac{d^2 \psi(x)}{dx^2} dx.$$

(b) When $|\phi\rangle$ and $|\psi\rangle$ are represented by $\phi(x, y, z)$ and $\psi(x, y, z)$, and $\hat{O} = \partial^2/\partial x^2$, we have

$$\langle \phi | \hat{O} | \psi \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi^*(x, y, z) \frac{\partial^2 \psi(x, y, z)}{\partial x^2} dx dy dz.$$

(c) When

$$|\phi\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}, \quad |\psi\rangle = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad \text{and} \quad \hat{O} = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix},$$

we have

$$\langle \phi | \hat{O} | \psi \rangle = [a_1^* \ a_2^*] \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}.$$

Comment Case (a) arises in 1-D wave mechanics. Case (b) arises in 3-D wave mechanics. Case (c) arises when describing the spin behaviour of a spin-half particle. Dirac brackets have the merit of providing a uniform notation for all these cases, but explicit calculations generally require us to interpret the Dirac brackets according to context – as integrals or matrix products.

Topic 2 — Hermitian operators

Solution 2.1 A Hermitian operator \hat{A} is an operator that obeys

$$\langle \phi | \hat{A} \psi \rangle = \langle \hat{A} \phi | \psi \rangle \quad \text{for all normalizable } \phi \text{ and } \psi.$$

Integrating both sides of the given identity from $-\infty$ to $+\infty$ gives

$$\left[\psi^*(x) \frac{d\phi}{dx} - \frac{d\psi^*}{dx} \phi(x) \right]_{-\infty}^{\infty} = \int_{-\infty}^{\infty} \psi^*(x) \frac{d^2 \phi}{dx^2} dx - \int_{-\infty}^{\infty} \frac{d^2 \psi^*}{dx^2} \phi(x) dx.$$

If the functions $\psi(x)$ and $\phi(x)$ are normalizable, these functions vanish at infinity, so the left-hand side is equal to zero. Hence

$$\int_{-\infty}^{\infty} \psi^*(x) \frac{d^2 \phi}{dx^2} dx = \int_{-\infty}^{\infty} \left(\frac{d^2 \psi^*}{dx^2} \right) \phi(x) dx = \int_{-\infty}^{\infty} \left(\frac{d^2 \psi}{dx^2} \right)^* \phi(x) dx$$

for any normalizable $\psi(x)$ and $\phi(x)$. This is just the Hermitian condition:

$$\left\langle \psi \left| \frac{d^2 \phi}{dx^2} \right. \right\rangle = \left\langle \frac{d^2 \psi}{dx^2} \left| \phi \right. \right\rangle$$

for the operator d^2/dx^2 .

Comment In one dimension, the kinetic energy operator is $-(\hbar^2/2m) d^2/dx^2$. This is a real constant times d^2/dx^2 , so the Hermitian nature of d^2/dx^2 implies that the kinetic energy operator is Hermitian. This makes good sense because kinetic energy is an observable quantity.

Solution 2.2 If ψ and ϕ are normalizable functions and \hat{A} and \hat{B} are Hermitian operators,

$$\begin{aligned} \langle \phi | \hat{C} \psi \rangle &\equiv \langle \phi | \hat{A} \hat{B} \hat{A} \psi \rangle \\ &= \langle \phi | \hat{A} (\hat{B} \hat{A} \psi) \rangle \\ &= \langle \hat{A} \phi | \hat{B} \hat{A} \psi \rangle \quad \text{since } \hat{A} \text{ is Hermitian} \\ &= \langle \hat{A} \phi | \hat{B} (\hat{A} \psi) \rangle \\ &= \langle \hat{B} \hat{A} \phi | \hat{A} \psi \rangle \quad \text{since } \hat{B} \text{ is Hermitian} \\ &= \langle \hat{A} \hat{B} \hat{A} \phi | \psi \rangle \quad \text{since } \hat{A} \text{ is Hermitian} \\ &\equiv \langle \hat{C} \phi | \psi \rangle. \end{aligned}$$

Comment We are told that ψ is normalizable, but have actually used something slightly beyond this. In order to use the Hermitian property in intermediate steps, we have implicitly assumed that $\hat{B}\hat{A}\psi$ and $\hat{A}\psi$ are also normalizable. At this level, such mathematical niceties are generally ignored without comment. The reason is pragmatic – a vast amount of mathematical theory and effort would be needed to be completely rigorous about this, far beyond the scope of undergraduate physics, and there is little to gain for nearly all practical purposes.

Solution 2.3 We have

$$\begin{aligned}
\langle \phi | \hat{A} \hat{B} | \psi \rangle &\equiv \langle \phi | \hat{A} \hat{B} \psi \rangle \\
&= \langle \hat{A} \phi | \hat{B} \psi \rangle \quad \text{since } \hat{A} \text{ is Hermitian} \\
&= \langle \hat{B} \hat{A} \phi | \psi \rangle \quad \text{since } \hat{B} \text{ is Hermitian} \\
&= \langle \psi | \hat{B} \hat{A} \phi \rangle^* \quad \text{using a general property of Dirac brackets.} \\
&\equiv \langle \psi | \hat{B} \hat{A} | \psi \rangle^*.
\end{aligned}$$

Comment It is important to respect the ordering in a product of operators (unless they are known to commute with one another). An expression like $\langle \phi | \hat{A} \hat{B} \psi \rangle$ is interpreted as $\langle \phi | \hat{A}(\hat{B}\psi) \rangle$, so the Hermitian property is applied first to \hat{A} and then to \hat{B} .

Solution 2.4 Given that $|\psi\rangle = \sum_n c_n |\phi_n\rangle$, we have $\langle \psi | = \sum_n c_n^* \langle \phi_n |$, so

$$\begin{aligned}
\langle \psi | \hat{A} | \psi \rangle &= \sum_m \sum_n c_m^* c_n \langle \phi_m | \hat{A} | \phi_n \rangle \\
&= \sum_m \sum_n c_m^* c_n \langle \phi_m | a_n | \phi_n \rangle \\
&= \sum_m \sum_n c_m^* c_n a_n \langle \phi_m | \phi_n \rangle,
\end{aligned}$$

where we have used the eigenvalue equation $\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle$.

Because \hat{A} is a Hermitian operator, its eigenvectors, corresponding to different eigenvalues, are orthogonal. Hence

$$\langle \psi | \hat{A} | \psi \rangle = \sum_m \sum_n c_m^* c_n a_n \delta_{mn} = \sum_n c_n^* c_n a_n,$$

as required.

Comments (1) We were careful to use different indices (m and n) for the two sums inserted into $\langle \psi | \hat{A} | \psi \rangle$. This is to avoid omitting cross-product terms.

(2) The mathematical result derived here has an important consequence in quantum mechanics. Both sides of the expression represent the expectation value of the observable A in the state $|\psi\rangle$. The left-hand side evaluates this expectation value using the sandwich rule while the right-hand side uses $\langle A \rangle = \sum_n p_n a_n$, where $p_n = |c_n|^2$ according to the coefficient rule.

Solution 2.5 The expectation value of A in the state Ψ is

$$\begin{aligned}
\langle A \rangle &= \langle \Psi | \hat{A} | \Psi \rangle \\
&= \langle \Psi | \hat{A} \Psi \rangle \\
&= \langle \hat{A} \Psi | \Psi \rangle \quad \text{because } \hat{A} \text{ is Hermitian} \\
&= \langle \Psi | \hat{A} \Psi \rangle^* \quad \text{from a general property of Dirac brackets} \\
&= \langle \Psi | \hat{A} | \Psi \rangle^* \\
&= \langle A \rangle^*.
\end{aligned}$$

Any quantity that is equal to its own complex conjugate is real, so $\langle A \rangle$ is real.

Comment As all measured values are real numbers, the expectation value of any observable must be real. The above calculation shows that quantum mechanics is consistent with this obvious fact because all observables are represented by Hermitian operators.

Topic 3 — Commutators and generalized Ehrenfest theorem

Solution 3.1 Since \hat{A} commutes with \hat{H} , the generalized Ehrenfest theorem gives

$$\frac{d\langle A \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle = 0.$$

Also, since \hat{A} commutes with \hat{H} , we have $\hat{A}\hat{H} = \hat{H}\hat{A}$ allowing us to write

$$\begin{aligned} [\hat{A}^2, \hat{H}] &= \hat{A}\hat{A}\hat{H} - \hat{H}\hat{A}\hat{A} \\ &= \hat{A}\hat{H}\hat{A} - \hat{A}\hat{H}\hat{A} = 0. \end{aligned}$$

So the generalized Ehrenfest theorem gives

$$\frac{d\langle A^2 \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{A}^2, \hat{H}] \rangle = 0.$$

Consequently,

$$\begin{aligned} \frac{d(\Delta A)^2}{dt} &= \frac{d}{dt} \left(\langle A^2 \rangle - \langle A \rangle^2 \right) \\ &= \frac{d\langle A^2 \rangle}{dt} - \frac{d\langle A \rangle^2}{dt} \\ &= \frac{d\langle A^2 \rangle}{dt} - 2\langle A \rangle \frac{d\langle A \rangle}{dt} = 0, \end{aligned}$$

from our previous results for $d\langle A \rangle/dt$ and $d\langle A^2 \rangle/dt$.

Comment Calculations similar to these show that $\langle A^3 \rangle, \langle A^4 \rangle \dots$ and so on remain constant in time. Although not proven here, it is also possible to show that, when \hat{A} commutes with \hat{H} , the entire probability distribution for the values of A remains constant in time. For example, the probability distribution for the momentum of a free particle remains constant in time because the momentum operator \hat{p}_x commutes with the Hamiltonian operator $\hat{p}_x^2/2m$ of a free particle. The same cannot be said of the probability distribution for the position of a free particle because the position operator \hat{x} does not commute with $\hat{p}_x^2/2m$.

Solution 3.2 (a) We have

$$\langle \psi_n | [\hat{A}, \hat{H}] | \psi_n \rangle = \langle \psi_n | \hat{A}\hat{H} | \psi_n \rangle - \langle \psi_n | \hat{H}\hat{A} | \psi_n \rangle.$$

The operator \hat{H} is Hermitian because it represents an observable quantity (energy). Using the Hermitian property of \hat{H} and the fact that $|\phi_n\rangle$ is an eigenvector of \hat{H} with eigenvalue E_n , we obtain

$$\begin{aligned} \langle \psi_n | [\hat{A}, \hat{H}] | \psi_n \rangle &= \langle \psi_n | \hat{A} | \hat{H} \psi_n \rangle - \langle \hat{H} \psi_n | \hat{A} | \psi_n \rangle \\ &= \langle \psi_n | \hat{A} | E_n \psi_n \rangle - \langle E_n \psi_n | \hat{A} | \psi_n \rangle \\ &= (E_n - E_n^*) \langle \psi_n | \hat{A} | \psi_n \rangle, \end{aligned}$$

and this is equal to zero because the Hermitian operator \hat{H} has real eigenvalues, giving $E_n - E_n^* = 0$.

(b) The generalized Ehrenfest theorem tells us that

$$\frac{d\langle A \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle.$$

Part (a) showed that the expectation value of the commutator on the right-hand side is equal to zero in an energy eigenstate. It follows that the left-hand side is also equal to zero in such a state.

Comment Note that this result differs from that of Exercise 3.1. The present result refers to any operator \hat{A} in a special type of state – an energy eigenstate (a stationary state). By contrast, Exercise 3.1 referred to a special type of operator (one that commutes with the Hamiltonian operator), but the state of the system was arbitrary.

Solution 3.3 The generalized Ehrenfest theorem tells us that

$$\frac{d\langle p_z \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{p}_z, \hat{H}] \rangle.$$

Since \hat{p}_z is a constant times $\partial/\partial z$, it commutes with all the momentum component operators and their squares and it also commutes with the operators \hat{x} and \hat{y} and their squares. We therefore have

$$[\hat{p}_z, \hat{p}_x^2] = [\hat{p}_z, \hat{p}_y^2] = [\hat{p}_z, \hat{p}_z^2] = [\hat{p}_z, \hat{x}^2] = [\hat{p}_z, \hat{y}^2] = 0,$$

so

$$[\hat{p}_z, \hat{H}] = 0,$$

and hence

$$\frac{d\langle p_z \rangle}{dt} = 0.$$

Comments (1) This is an example of a symmetry leading to a conservation law. The fact that the potential energy function does not depend on z is a symmetry. This leads to the conservation of $\langle p_z \rangle$, the expectation value of the z -component of momentum.

(2) An analogous situation arises in classical physics, where the absence of a force in the z -direction leads to the conservation of p_z .

Solution 3.4 We have

$$\begin{aligned} [\hat{p}_x, \hat{x}^2] f(x) &= (\hat{p}_x \hat{x}^2 - \hat{x}^2 \hat{p}_x) f(x) \\ &= -i\hbar \left(\frac{\partial}{\partial x} (x^2 f(x)) - x^2 \frac{\partial f}{\partial x} \right) \\ &= -i\hbar \left(2x f(x) + x^2 \frac{\partial f}{\partial x} - x^2 \frac{\partial f}{\partial x} \right) \\ &= -2i\hbar x f(x). \end{aligned}$$

Since this is true for any $f(x)$, we have

$$[\hat{p}_x, \hat{x}^2] = -2i\hbar \hat{x}.$$

For a particle of mass m , subject to the potential energy function $V(x) = \frac{1}{2}Cx^2$, the generalized Ehrenfest theorem then gives

$$\frac{d\langle p_x \rangle}{dt} = \frac{1}{i\hbar} \left\langle \left[\hat{p}_x, \frac{\hat{p}_x^2}{2m} + \frac{1}{2}C\hat{x}^2 \right] \right\rangle$$

Using $[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$ and the fact that $[\hat{p}_x, \hat{p}_x^2] = 0$, we have

$$\begin{aligned} \frac{d\langle p_x \rangle}{dt} &= \frac{C}{2i\hbar} \langle [\hat{p}_x, \hat{x}^2] \rangle \\ &= \frac{C}{2i\hbar} \times \langle -2i\hbar x \rangle \\ &= -C \langle x \rangle. \end{aligned}$$

Comments (1) In wave mechanics, any commutator is an operator that acts on functions. To simplify a commutator, it is a good idea to let the commutator act on an arbitrary function – for example, $f(x)$ or $f(x, y, z)$ depending on the context. We then expand the expression into separate terms and carry out any differentiations

that arise. The interesting differentiations involve products of position-dependent factors in the commutator with the arbitrary function f , as these produce terms that do not cancel out. The simplified result is expressed as an operator acting on f . Because the function f is arbitrary, we omit it from the final answer, giving an identity between operators.

(2) The result established here is the quantum-mechanical analogue of Newton's second law for a harmonic oscillator. This is not exactly the same as Newton's second law because it involves expectation values, but the analogy is close.

Solution 3.5 For any function, $f(x)$, we have

$$\begin{aligned} (\hat{x}\hat{p}_x^2 - \hat{p}_x^2\hat{x})f(x) &= -\hbar^2 \left(x\frac{\partial^2 f}{\partial x^2} - \frac{\partial^2}{\partial x^2}(xf(x)) \right) \\ &= -\hbar^2 \left(x\frac{\partial^2 f}{\partial x^2} - \frac{\partial}{\partial x} \left(f(x) + x\frac{\partial f}{\partial x} \right) \right) \\ &= -\hbar^2 \left(x\frac{\partial^2 f}{\partial x^2} - \left(2\frac{\partial f}{\partial x} + x\frac{\partial^2 f}{\partial x^2} \right) \right) \\ &= 2\hbar^2 \frac{\partial f}{\partial x} \\ &= 2i\hbar \left(-i\hbar \frac{\partial f}{\partial x} \right). \end{aligned}$$

Since this is true for any $f(x)$, we can finally use $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ to obtain the operator equation

$$[\hat{x}, \hat{p}_x^2] = 2i\hbar \hat{p}_x.$$

The generalized Ehrenfest theorem then gives

$$\begin{aligned} \frac{d\langle x \rangle}{dt} &= \frac{1}{i\hbar} \left\langle [\hat{x}, \frac{\hat{p}_x^2}{2m} + \hat{V}(x)] \right\rangle \\ &= \frac{1}{2mi\hbar} \langle [\hat{x}, \hat{p}_x^2] \rangle \quad \text{since } [\hat{x}, \hat{V}(x)] = 0 \\ &= \frac{1}{2mi\hbar} \times \langle 2i\hbar p_x \rangle \\ &= \frac{\langle p_x \rangle}{m}. \end{aligned}$$

Comment This is the quantum-mechanical analogue of the familiar classical relationship between momentum and velocity. Note, however that the quantum-mechanical result involves expectation values. We can never say that $dx/dt = p_x/m$ in quantum mechanics because x and p_x do not both have definite values in the same state.

Solution 3.6 (a) For an arbitrary function $f(x)$, we have

$$\begin{aligned} [\hat{p}_x, V(x)]f(x) &= \hat{p}_x V(x)f(x) - V(x)\hat{p}_x f(x) \\ &= -i\hbar \left(\frac{d}{dx}(V(x)f(x)) - V(x)\frac{df}{dx} \right) \\ &= -i\hbar \left(\frac{dV}{dx}f(x) + V(x)\frac{df}{dx} - V(x)\frac{df}{dx} \right) \\ &= -i\hbar \frac{dV}{dx}f(x). \end{aligned}$$

Since this equation is true for an arbitrary function $f(x)$, we have the operator equation

$$[\hat{p}_x, V(x)] = -i\hbar \frac{dV}{dx}.$$

(b) We consider the expression

$$\hat{X} = \hat{p}_x [\hat{p}_x, V(x)] + [\hat{p}_x, V(x)] \hat{p}_x.$$

Expanding the commutators gives

$$\begin{aligned}\hat{X} &= \hat{p}_x (\hat{p}_x V(x) - V(x) \hat{p}_x) + (\hat{p}_x V(x) - V(x) \hat{p}_x) \hat{p}_x \\ &= \hat{p}_x^2 V(x) - V(x) \hat{p}_x^2 \\ &= [\hat{p}_x^2, V(x)].\end{aligned}$$

On the other hand, using the result of part (a),

$$\begin{aligned}\hat{X} &= \hat{p}_x \left(-i\hbar \frac{dV}{dx} \right) + \left(-i\hbar \frac{dV}{dx} \right) \hat{p}_x \\ &= -i\hbar \left(\hat{p}_x \frac{dV}{dx} + \frac{dV}{dx} \hat{p}_x \right).\end{aligned}$$

Comparing these two expressions for \hat{X} , we conclude that

$$[\hat{p}_x^2, V(x)] = -i\hbar \left(\hat{p}_x \frac{dV}{dx} + \frac{dV}{dx} \hat{p}_x \right).$$

Comment It is very important to respect the order of operators that do not commute. Our final answer cannot be further simplified for a general $V(x)$ because \hat{p}_x does not commute with any non-constant function of x .

Solution 3.7 The generalized Ehrenfest theorem tells us that

$$\frac{d\langle E_{\text{kin}} \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{E}_{\text{kin}}, \hat{H}] \rangle,$$

where the Hamiltonian operator \hat{H} is a sum of kinetic and potential energy terms: $\hat{H} = \hat{E}_{\text{kin}} + \hat{V}$. The kinetic energy operator commutes with itself, so

$$[\hat{E}_{\text{kin}}, \hat{H}] = [\hat{E}_{\text{kin}}, \hat{V}] = \frac{1}{2m} [\hat{p}_x^2, \hat{V}].$$

Using the result of Exercise 3.6(b), we conclude that

$$\frac{d\langle E_{\text{kin}} \rangle}{dt} = -\frac{1}{2m} \left(\hat{p}_x \frac{dV}{dx} + \frac{dV}{dx} \hat{p}_x \right).$$

In the special case $V(x) = mgx$, we have $dV/dx = mg$, which commutes with \hat{p}_x , and so

$$\frac{d\langle E_{\text{kin}} \rangle}{dt} = -\frac{1}{2m} \langle 2mg\hat{p}_x \rangle = -g\langle p_x \rangle.$$

Comment With the x -axis pointing vertically upwards, the given potential energy function is that for gravity close to the Earth's surface. Our answer shows that $\langle E_{\text{kin}} \rangle$ decreases when $\langle p_x \rangle > 0$ and $\langle E_{\text{kin}} \rangle$ increases when $\langle p_x \rangle < 0$. These results agree with our classical experience of watching a ball rise and fall after being thrown vertically upwards.

Topic 4 — Orbital angular momentum

Solution 4.1 In the present context, the generalized uncertainty principle tells us that

$$\Delta L_x \Delta L_y \geq \frac{1}{2} \left| \langle [\hat{L}_x, \hat{L}_y] \rangle \right|.$$

Using the standard commutation relations for orbital angular momentum, this gives

$$\Delta L_x \Delta L_y = \frac{1}{2} \left| \langle i\hbar \hat{L}_z \rangle \right|,$$

so

$$\Delta L_x \Delta L_y \geq \frac{\hbar}{2} |\langle L_z \rangle|.$$

If the system is in a state with a definite non-zero value of L_z , the right-hand side of this equation is greater than (not equal to) zero. So both ΔL_x and ΔL_y are non-zero, and this implies that neither L_x nor L_y have definite values in this state.

Comment It is possible for L_x , L_y and L_z to all be equal to *zero* in the same state. In fact, this happens in the ground state of a hydrogen atom. However, it is not possible for any two of these quantities to have definite *non-zero* values in the same state. We say that L_x , L_y and L_z are incompatible observables. The hallmark of a set of incompatible observables is that they are represented by operators that do not commute with one another.

Solution 4.2 In classical physics, the inhomogeneous magnetic field in a Stern–Gerlach apparatus deflects a silver atom according to the component of the atom’s magnetic moment along an axis of symmetry joining the Stern–Gerlach pole pieces. The distinct traces in the Stern–Gerlach experiment reveal a quantization of this component of magnetic moment. Assuming that the magnetic moment is associated with an angular momentum, we can conclude that the angular momentum component along the axis of symmetry joining the pole pieces is quantized.

The number of different values of a component of orbital angular momentum is $2l + 1$, where l is the orbital angular momentum quantum number, which is a non-negative integer ($l = 0, 1, 2, \dots$). This implies that an odd number of distinct traces should be detected (1 or 3 or 5 \dots). The fact that *two* traces are detected cannot be explained in terms of *orbital* angular momentum.

Comment In order to explain the existence of *two* traces, we need the concept of spin. In its ground state, a silver atom has $l = 0$, but it also has a net spin angular momentum characterized by the spin quantum number $s = \frac{1}{2}$. This gives rise to $(2s + 1) = 2$ traces, corresponding to $S_z = +\hbar/2$ and $S_z = -\hbar/2$, where the z -direction is the axis of symmetry joining the pole pieces.

Solution 4.3 We have

$$x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi \quad \text{and} \quad z = r \cos \theta$$

so

$$\begin{aligned} V &= C_1 r^2 \sin^2 \theta (\cos^2 \phi + \sin^2 \phi) + C_2 r^2 \cos^2 \theta \\ &= C_1 r^2 \sin^2 \theta + C_2 r^2 \cos^2 \theta. \end{aligned}$$

Since \hat{V} does not depend on ϕ , the operator $\hat{L}_z = -i\hbar \partial/\partial\phi$ commutes with the potential energy term in the Hamiltonian operator. The question states that \hat{L}_z commutes with $\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2$, so \hat{L}_z also commutes with the kinetic energy term $(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2)/2m$. Hence, \hat{L}_z commutes with the Hamiltonian operator, \hat{H} . The generalized Ehrenfest theorem then tells us that

$$\frac{d\langle L_z \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{L}_z, \hat{H}] \rangle = 0.$$

Comments (1) This is another example of symmetry leading to a conservation law. In this case, the potential energy function is unaffected by rotations around the z -axis (in spherical coordinates, it does not depend on the azimuthal angle, ϕ). This leads to the conservation of $\langle L_z \rangle$, the expectation value of the z -component of angular momentum.

(2) An analogous situation arises in classical physics, where the absence of a torque in the z -direction leads to the conservation of L_z .

Solution 4.4 In the state $|l, m\rangle$ we have

$$\hat{L}^2 |l, m\rangle = l(l+1)\hbar^2 |l, m\rangle \quad \text{and} \quad \hat{L}_z |l, m\rangle = m\hbar |l, m\rangle \quad \text{so} \quad \hat{L}_z^2 |l, m\rangle = m^2 \hbar^2 |l, m\rangle$$

and

$$(\hat{L}_x^2 + \hat{L}_y^2) |l, m\rangle = (\hat{L}^2 - \hat{L}_z^2) |l, m\rangle = (l(l+1)\hbar^2 - m^2 \hbar^2) |l, m\rangle.$$

Hence the value $(l(l+1) - m^2)\hbar^2$ is obtained with certainty.

Comment Although L_x and L_y do not have definite values in the state $|l, m\rangle$, the special combination $L_x^2 + L_y^2$ does have a definite value in this state because it can be expressed entirely in terms of L^2 and L_z , which have the definite values $l(l+1)\hbar^2$ and $m\hbar$.

Solution 4.5 Since $\hat{L}_z|\psi_m\rangle = m\hbar|\psi_m\rangle$, we have

$$\langle\psi_m|\hat{L}_y\hat{L}_z|\psi_m\rangle = m\hbar\langle\psi_m|\hat{L}_y|\psi_m\rangle.$$

Also, because \hat{L}_z is Hermitian and $m\hbar$ is real,

$$\langle\psi_m|\hat{L}_z\hat{L}_y|\psi_m\rangle = \langle\hat{L}_z\psi_m|\hat{L}_y|\psi_m\rangle = m\hbar\langle\psi_m|\hat{L}_y|\psi_m\rangle.$$

Comparing these results, we conclude that

$$\langle\psi_m|\hat{L}_y\hat{L}_z|\psi_m\rangle = \langle\psi_m|\hat{L}_z\hat{L}_y|\psi_m\rangle.$$

Hence,

$$\langle\psi_m|\hat{L}_y\hat{L}_z - \hat{L}_z\hat{L}_y|\psi_m\rangle = 0.$$

Using the commutation relations for angular momentum, we then have

$$0 = \langle\psi_m|\hat{L}_y\hat{L}_z - \hat{L}_z\hat{L}_y|\psi_m\rangle = \langle\psi_m|i\hbar\hat{L}_x|\psi_m\rangle = i\hbar\langle L_x\rangle.$$

So, in the state ψ_m , we have $\langle L_x\rangle = 0$.

Comment A similar argument, based on the standard commutation relation for \hat{L}_x and \hat{L}_z shows that $\langle L_y\rangle = 0$ in the state ψ_m .

Solution 4.6 In the state $|l, m\rangle$, the result of Exercise 4.4 gives

$$\langle L_x^2 + L_y^2 \rangle = (l(l+1) - m^2)\hbar^2.$$

Using the result $\langle L_x^2 \rangle = \langle L_y^2 \rangle$, we then have

$$\langle L_x^2 \rangle = \langle L_y^2 \rangle = \frac{1}{2}(l(l+1) - m^2)\hbar^2.$$

From Exercise 4.5 we also know that $\langle L_x \rangle = \langle L_y \rangle = 0$, so

$$\Delta L_x = (\langle L_x^2 \rangle - \langle L_x \rangle^2)^{1/2} = \frac{1}{\sqrt{2}}(l(l+1) - m^2)^{1/2}\hbar$$

$$\Delta L_y = (\langle L_y^2 \rangle - \langle L_y \rangle^2)^{1/2} = \frac{1}{\sqrt{2}}(l(l+1) - m^2)^{1/2}\hbar.$$

Also $\langle L_z \rangle = m\hbar$ and $\langle L_z^2 \rangle = m^2\hbar^2$, so

$$\Delta L_z = (\langle L_z^2 \rangle - \langle L_z \rangle^2)^{1/2} = 0.$$

For orbital angular momentum, the generalized uncertainty principle gives

$$\Delta L_x \Delta L_y \geq \frac{1}{2} \left| \langle [\hat{L}_x, \hat{L}_y] \rangle \right| = \frac{\hbar}{2} |\langle L_z \rangle|$$

$$\Delta L_y \Delta L_z \geq \frac{1}{2} \left| \langle [\hat{L}_y, \hat{L}_z] \rangle \right| = \frac{\hbar}{2} |\langle L_x \rangle|$$

$$\Delta L_z \Delta L_x \geq \frac{1}{2} \left| \langle [\hat{L}_z, \hat{L}_x] \rangle \right| = \frac{\hbar}{2} |\langle L_y \rangle|.$$

Substituting the above results into the first of these inequalities gives

$$\frac{1}{2}(l(l+1) - m^2)\hbar^2 \geq \frac{|m|\hbar^2}{2}.$$

which is true because $l \geq |m|$ so $l(l+1) - m^2 \geq |m|$. The other two uncertainty relations are satisfied in the form $0 \geq 0$.

Comment The question assumed that $\langle L_x^2 \rangle = \langle L_y^2 \rangle$ in the state $|l, m\rangle$. This result can be justified on symmetry grounds because the state $|l, m\rangle$ does not depend on the directions chosen for the x - and y -axes.

Topic 5 — Spin angular momentum

Solution 5.1 The spin states $|\uparrow_x\rangle$ and $|\uparrow_y\rangle$ are *not* orthogonal. One way of seeing this is to use the $\cos^2(\theta/2)$ rule. The angle between the x - and y -directions is 90° so, when the particle is in the spin state $|\uparrow_x\rangle$, the probability that a spin measurement in the y -direction will give a spin-up result is $\cos^2(90^\circ/2) = \frac{1}{2}$. This probability is also given by $|\langle\uparrow_y|\uparrow_x\rangle|^2$, so we can conclude that $\langle\uparrow_y|\uparrow_x\rangle \neq 0$.

Alternatively, we can use $|\uparrow_x\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $|\uparrow_y\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}$ to obtain

$$\langle\uparrow_y|\uparrow_x\rangle = \frac{1}{2} \begin{bmatrix} 1 & -i \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{2}(1 - i) \neq 0.$$

Comment We know that the x -direction is orthogonal to the y -direction, so it may come as a surprise that $|\uparrow_x\rangle$ is not orthogonal to $|\uparrow_y\rangle$. Although the x -direction is orthogonal to the y -direction in ordinary space, the non-orthogonality of $|\uparrow_x\rangle$ and $|\uparrow_y\rangle$ refers to vectors in spin space. These two spaces are not the same. Ordinary space is three-dimensional and its vectors have real components; spin space is two-dimensional and its vectors have complex components. The fact that $|\uparrow_x\rangle$ is not orthogonal to $|\uparrow_y\rangle$ tells us that a particle that is definitely spin-up in the x -direction has a non-zero probability of giving spin-up when its spin is measured in the y -direction. By contrast, $|\uparrow_x\rangle$ and $|\downarrow_x\rangle$ are orthogonal.

Solution 5.2 The x -direction corresponds to $\theta = \pi/2$ and $\phi = 0$, so

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}} (|\uparrow_z\rangle + |\downarrow_z\rangle).$$

The $\theta = 2\pi/3, \phi = \pi/2$ direction corresponds to

$$\cos(\theta/2) = \frac{1}{2}, \quad \sin(\theta/2) = \frac{\sqrt{3}}{2} \quad \text{and} \quad e^{i\phi} = i,$$

so the spin-up ket for spin-up in the \mathbf{n} -direction is

$$|\uparrow_{\mathbf{n}}\rangle = \frac{1}{2}|\uparrow_z\rangle + \frac{\sqrt{3}}{2}i|\downarrow_z\rangle.$$

The probability amplitude for measuring spin-up in the \mathbf{n} -direction in the state $|\uparrow_x\rangle$ is

$$\begin{aligned} \langle\uparrow_{\mathbf{n}}|\uparrow_x\rangle &= \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2}i \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \\ &= \frac{1}{2\sqrt{2}} - \frac{\sqrt{3}}{2\sqrt{2}}i, \end{aligned}$$

so the corresponding probability is

$$\text{probability} = \left| \frac{1}{2\sqrt{2}} - \frac{\sqrt{3}}{2\sqrt{2}}i \right|^2 = \frac{1}{8} + \frac{3}{8} = \frac{1}{2}.$$

Comment This agrees with the $\cos^2(\theta/2)$ rule because the angle between the x -direction and the \mathbf{n} -direction is 90° and $\cos^2(45^\circ) = 1/2$.

Solution 5.3 (a)(i) Let $|D\rangle = a_1|\uparrow_x\rangle + a_2|\downarrow_x\rangle$, then

$$a_1 = \langle\uparrow_x|D\rangle = \frac{1}{5\sqrt{2}} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \frac{7}{5\sqrt{2}}$$

$$a_2 = \langle\downarrow_x|D\rangle = \frac{1}{5\sqrt{2}} \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \frac{1}{5\sqrt{2}},$$

so

$$|D\rangle = \frac{1}{5\sqrt{2}} (7|\uparrow_x\rangle + |\downarrow_x\rangle).$$

(ii) Let $|D\rangle = b_1|\uparrow_y\rangle + b_2|\downarrow_y\rangle$, then

$$b_1 = \langle \uparrow_y |D\rangle = \frac{1}{5\sqrt{2}} [1 \ -i] \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \frac{3-4i}{5\sqrt{2}}$$

$$b_2 = \langle \downarrow_y |D\rangle = \frac{1}{5\sqrt{2}} [-i \ 1] \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \frac{-3i+4}{5\sqrt{2}},$$

so

$$|D\rangle = \frac{1}{5\sqrt{2}} ((3-4i)|\uparrow_y\rangle + (-3i+4)|\downarrow_y\rangle).$$

(iii) By inspection,

$$|D\rangle = \frac{1}{5} (3|\uparrow_z\rangle + 4|\downarrow_z\rangle).$$

(b) Using the coefficient rule, the probability of getting spin-up in the x -direction is

$$\left| \frac{7}{5\sqrt{2}} \right|^2 = \frac{49}{50}.$$

The probability of getting spin-up in the y -direction is

$$\left| \frac{3-4i}{5\sqrt{2}} \right|^2 = \frac{1}{2}.$$

The probability of getting spin-up in the z -direction is

$$\left| \frac{3}{5} \right|^2 = \frac{9}{25}.$$

Comment The components of the spinor $|D\rangle$ give the coefficients in the basis of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$. These coefficients are probability amplitudes so, by taking their modulus squared, we can find the probabilities for measuring spin-up and spin-down in the z -direction. The spinor $|D\rangle$ is a complete representation of the spin of a spin- $\frac{1}{2}$ particle, so probabilistic information about spin measured in other directions is implicit in it. For example, by taking the inner products $\langle \uparrow_x |D\rangle$ and $\langle \downarrow_x |D\rangle$, we can find the coefficients in the basis of $|\uparrow_x\rangle$ and $|\downarrow_x\rangle$. Taking the modulus squared of these coefficients gives the probabilities for measuring spin-up and spin-down in the x -direction.

Solution 5.4 In the given state we have

$$\begin{aligned} \langle S_x \rangle &= \langle A | \hat{S}_x | A \rangle \\ &= \frac{1}{\sqrt{5}} [1 \ -2i] \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2i \end{bmatrix} \\ &= \frac{\hbar}{10} [1 \ -2i] \begin{bmatrix} 2i \\ 1 \end{bmatrix} \\ &= \frac{\hbar}{10} (2i - 2i) = 0. \end{aligned}$$

$$\begin{aligned} \langle S_y \rangle &= \langle A | \hat{S}_y | A \rangle \\ &= \frac{1}{\sqrt{5}} [1 \ -2i] \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2i \end{bmatrix} \\ &= \frac{\hbar}{10} [1 \ -2i] \begin{bmatrix} 2 \\ i \end{bmatrix} \\ &= \frac{\hbar}{10} (2 + 2) = \frac{2}{5}\hbar. \end{aligned}$$

$$\begin{aligned}
\langle S_z \rangle &= \langle A | \hat{S}_z | A \rangle \\
&= \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & -2i \end{bmatrix} \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2i \end{bmatrix} \\
&= \frac{\hbar}{10} \begin{bmatrix} 1 & -2i \end{bmatrix} \begin{bmatrix} 1 \\ -2i \end{bmatrix} \\
&= \frac{\hbar}{10} (1 - 4) = -\frac{3}{10} \hbar.
\end{aligned}$$

Comment Given a spinor $|A\rangle$, the sandwich rule can be used to find the expectation value of a spin component measured in any direction. This involves evaluating the product of three matrices. Do not forget to take the complex conjugate of the components in $|A\rangle$ when forming $\langle A|$.

Solution 5.5 In the given state we have

$$\langle S_x \rangle = [a_1^* \ a_2^*] \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

$$= \frac{\hbar}{2} [a_1^* \ a_2^*] \begin{bmatrix} a_2 \\ a_1 \end{bmatrix}$$

$$= \frac{\hbar}{2} (a_1^* a_2 + a_2^* a_1).$$

$$\langle S_y \rangle = [a_1^* \ a_2^*] \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

$$= \frac{\hbar}{2} [a_1^* \ a_2^*] \begin{bmatrix} -ia_2 \\ ia_1 \end{bmatrix}$$

$$= -i \frac{\hbar}{2} (a_1^* a_2 - a_2^* a_1).$$

$$\langle S_z \rangle = [a_1^* \ a_2^*] \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

$$= \frac{\hbar}{2} [a_1^* \ a_2^*] \begin{bmatrix} a_1 \\ -a_2 \end{bmatrix}$$

$$= \frac{\hbar}{2} (a_1^* a_1 - a_2^* a_2).$$

Hence

$$\begin{aligned}
\langle S_x \rangle^2 + \langle S_y \rangle^2 + \langle S_z \rangle^2 &= \frac{\hbar^2}{4} [(a_1^* a_2 + a_2^* a_1)^2 - (a_1^* a_2 - a_2^* a_1)^2 + (a_1^* a_1 - a_2^* a_2)^2] \\
&= \frac{\hbar^2}{4} [4a_1^* a_2 a_2^* a_1 + (a_1^* a_1 - a_2^* a_2)^2] \\
&= \frac{\hbar^2}{4} (a_1^* a_1 + a_2^* a_2)^2 \\
&= \frac{\hbar^2}{4} (|a_1|^2 + |a_2|^2)^2 \\
&= \frac{\hbar^2}{4}
\end{aligned}$$

because the spin state is normalized.

Comments (1) We are free to choose the z -axis in any way we like and can choose it to point in the direction along which the particle is certain to give spin-up. In this special case, we have $\langle S_z \rangle = \hbar/2$, $\langle S_x \rangle = 0$ and

$\langle S_y \rangle = 0$, so the formula derived above is true for this special choice of coordinate system. The above derivation confirms that the formula does not depend on our choice of axes, just as we would expect.

(2) The answer to Exercise 5.4 agrees with the result derived here because $0^2 + (2\hbar/5)^2 + (-3\hbar/10)^2 = \hbar^2/4$.

Solution 5.6 We have

$$\begin{aligned}
 \langle \uparrow_{\mathbf{n}} | \hat{S}_x | \uparrow_{\mathbf{n}} \rangle &= [\cos(\theta/2) \quad \sin(\theta/2)e^{-i\phi}] \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{bmatrix} \\
 &= \frac{\hbar}{2} [\cos(\theta/2) \quad \sin(\theta/2)e^{-i\phi}] \begin{bmatrix} \sin(\theta/2)e^{i\phi} \\ \cos(\theta/2) \end{bmatrix} \\
 &= \frac{\hbar}{2} \cos(\theta/2) \sin(\theta/2) (e^{i\phi} + e^{-i\phi}) \\
 &= \frac{\hbar}{2} \cos(\theta/2) \sin(\theta/2) (2 \cos \phi) \\
 &= \frac{\hbar}{2} \sin \theta \cos \phi,
 \end{aligned}$$

where we have used $\sin(2\theta) = 2 \sin(\theta) \cos(\theta)$ with θ replaced by $\theta/2$.

Also,

$$\begin{aligned}
 \langle \uparrow_{\mathbf{n}} | \hat{S}_y | \uparrow_{\mathbf{n}} \rangle &= [\cos(\theta/2) \quad \sin(\theta/2)e^{-i\phi}] \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{bmatrix} \\
 &= \frac{\hbar}{2} [\cos(\theta/2) \quad \sin(\theta/2)e^{-i\phi}] \begin{bmatrix} -i \sin(\theta/2)e^{i\phi} \\ i \cos(\theta/2) \end{bmatrix} \\
 &= \frac{\hbar}{2} \cos(\theta/2) \sin(\theta/2) (-ie^{i\phi} + ie^{-i\phi}) \\
 &= \frac{\hbar}{2} \cos(\theta/2) \sin(\theta/2) (2 \sin \phi) \\
 &= \frac{\hbar}{2} \sin \theta \sin \phi.
 \end{aligned}$$

Finally,

$$\begin{aligned}
 \langle \uparrow_{\mathbf{n}} | \hat{S}_z | \uparrow_{\mathbf{n}} \rangle &= [\cos(\theta/2) \quad \sin(\theta/2)e^{-i\phi}] \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{bmatrix} \\
 &= \frac{\hbar}{2} [\cos(\theta/2) \quad \sin(\theta/2)e^{-i\phi}] \begin{bmatrix} \cos(\theta/2) \\ -\sin(\theta/2)e^{i\phi} \end{bmatrix} \\
 &= \frac{\hbar}{2} (\cos^2(\theta/2) - \sin^2(\theta/2)) \\
 &= \frac{\hbar}{2} \cos \theta,
 \end{aligned}$$

where we have used $\cos(2\theta) = \cos^2(\theta) - \sin^2(\theta)$ with θ replaced by $\theta/2$.

Comment In classical physics, a vector \mathbf{a} , pointing in the direction $\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, has components

$$a_x = |a| \sin \theta \cos \phi, \quad a_y = |a| \sin \theta \sin \phi \quad \text{and} \quad a_z = |a| \cos \theta.$$

The result derived above is as close as we can get to the classical result. In quantum mechanics the three spin components S_x , S_y and S_z of a spin- $\frac{1}{2}$ particle are incompatible observables, so they do not all have definite values in the same state. But, if the particle is in a state that definitely gives spin-up when its spin is measured in the \mathbf{n} -direction, the *expectation values* $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$ obey formulas similar to those for the components of a classical vector. This sometimes gives us a quick way of finding the expectation value of a spin component, but this shortcut is not safe to use in an exam or assignment because marks will generally be allocated for explicit calculations like those in Exercise 5.4.

Solution 5.7 We have

$$\begin{aligned} i\hbar \frac{d}{dt} |A\rangle &= i\hbar \frac{d}{dt} \left(\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} e^{i\gamma_s B t/2} \right) \\ &= i\hbar \frac{i\gamma_s B}{2} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} e^{i\gamma_s B t/2} \\ &= -\frac{\gamma_s B \hbar}{2} |A\rangle. \end{aligned}$$

Also

$$\begin{aligned} \hat{H}|A\rangle &= -\frac{\gamma_s B \hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} e^{i\gamma_s B t/2} \\ &= -\frac{\gamma_s B \hbar}{2} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} e^{i\gamma_s B t/2} \\ &= -\frac{\gamma_s B \hbar}{2} |A\rangle, \end{aligned}$$

so

$$i\hbar \frac{d}{dt} |A\rangle = \hat{H}|A\rangle,$$

which confirms that $|A\rangle$ satisfies Schrödinger's equation.

Comment The spinor $|A_0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}$ is an eigenvector of the Hamiltonian matrix with eigenvalue $E = -\gamma_s B \hbar/2$, so the given state has the typical form of a stationary state:

$$|A\rangle = |A_0\rangle e^{-iEt/\hbar}.$$

Solution 5.8 At time $t \geq 0$, the spin ket describing the spin state of the particle is

$$|A\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow_n\rangle e^{-iE_u t/\hbar} + |\downarrow_n\rangle e^{-iE_d t/\hbar} \right)$$

where E_u is the energy eigenvalue corresponding to $|\uparrow_n\rangle$ and E_d is the energy eigenvalue corresponding to $|\downarrow_n\rangle$.

We have

$$\hat{H}|\uparrow_n\rangle = -\gamma_s B \hat{S}_n |\uparrow_n\rangle = -\gamma_s B \frac{\hbar}{2} |\uparrow_n\rangle = \frac{\hbar\omega}{2} |\uparrow_n\rangle,$$

where $\omega = -\gamma_s B$ is the Larmor frequency. Consequently, $E_u = \hbar\omega/2$. A similar argument with $|\downarrow_n\rangle$ gives $E_d = -\hbar\omega/2$. Hence

$$|A\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow_n\rangle e^{-i\omega t/2} + |\downarrow_n\rangle e^{+i\omega t/2} \right).$$

Comments (1) With the magnetic field in the n -direction, we express the initial spinor in terms of $|\uparrow_n\rangle$ and $|\downarrow_n\rangle$. The spin state at a later time is then obtained by introducing appropriate phase factors $e^{-iE_u t/\hbar}$ and $e^{-iE_d t/\hbar}$ to accompany $|\uparrow_n\rangle$ and $|\downarrow_n\rangle$. Here, E_u and E_d are the energy eigenvalues corresponding to spin-up and spin-down states in the n -direction (the direction of the magnetic field).

(2) It is essential to use the correct signs for E_u and E_d . When $\gamma_s < 0$, the spin-up eigenvalue E_u has the positive value $\hbar\omega/2$ where $\omega = -\gamma_s B \hbar/2 > 0$ is the Larmor frequency. By contrast when $\gamma_s > 0$, E_u has the negative value $-\hbar\omega/2$ where $\omega = \gamma_s B \hbar/2 > 0$ is the Larmor frequency.

Topic 6 — Many-particle systems

Solution 6.1 We have

$$\begin{aligned}
\hat{S}|A\rangle &= \left(\hat{S}_{z,1} + \hat{S}_{z,2}\right)|\uparrow\rangle_1|\uparrow\rangle_2 \\
&= \left(\hat{S}_{z,1}|\uparrow\rangle_1\right)|\uparrow\rangle_2 + |\uparrow\rangle_1\left(\hat{S}_{z,2}|\uparrow\rangle_2\right) \\
&= \left(\frac{\hbar}{2}|\uparrow\rangle_1\right)|\uparrow\rangle_2 + |\uparrow\rangle_1\left(\frac{\hbar}{2}|\uparrow\rangle_2\right) \\
&= \hbar|\uparrow\rangle_1|\uparrow\rangle_2
\end{aligned}$$

so $|A\rangle$ is an eigenvector of $\hat{S}_{z,1} + \hat{S}_{z,2}$, with eigenvalue \hbar .

Comment Note that the operator $\hat{S}_{z,1}$ acts only on the spin ket referring to particle 1, while the operator $\hat{S}_{z,2}$ acts only on the spin ket referring to particle 2.

Solution 6.2 In the ground state, both particles are in the lowest ($n = 1$) states, so at time $t = 0$ the normalized spatial wave function inside the well is

$$\frac{2}{L} \sin\left(\frac{\pi x_1}{L}\right) \sin\left(\frac{\pi x_2}{L}\right).$$

This is a symmetrical function of x_1 and x_2 . Since the particles have spin- $\frac{1}{2}$, they are fermions and have an antisymmetric total wave function, so the accompanying spin ket must be antisymmetric and is given by

$$|S = 0, M_S = 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$$

The normalized total wave function is therefore

$$\frac{\sqrt{2}}{L} \sin\left(\frac{\pi x_1}{L}\right) \sin\left(\frac{\pi x_2}{L}\right) (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

for $0 \leq x_1 \leq L$ and $0 \leq x_2 \leq L$, and vanishes outside this range.

Comments (1) In questions of this type, we first check that the particles are identical. If they are, we decide whether they are fermions or bosons. In this question, the two particles are identical and each is a fermion because it has spin- $\frac{1}{2}$. This system of identical fermions must have an antisymmetric total wave function.

(2) In the ground state of the two-particle system, both particles are in the spatial state ψ_1 . (This is consistent with the Pauli exclusion principle because the particles can have different spins.) It follows that the two-particle spatial state is symmetric. The two-particle spin state must therefore be antisymmetric in order to give an antisymmetric total wave function.

Solution 6.3 We have

$$|\uparrow\uparrow\rangle = |S = 1, M_S = 1\rangle$$

so

$$\begin{aligned}
\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 |\uparrow\uparrow\rangle &= \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 |S = 1, M_S = 1\rangle \\
&= \frac{1}{2} \left(\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2 \right) |S = 1, M_S = 1\rangle \\
&= \frac{1}{2} (S(S+1)\hbar^2 - s_1(s_1+1)\hbar^2 - s_2(s_2+1)\hbar^2) |S = 1, M_S = 1\rangle
\end{aligned}$$

where S is the total spin quantum number for the system and s_1 and s_2 are the spin quantum numbers for the individual particles (with $s_1 = s_2 = 1/2$). Hence,

$$\begin{aligned}
\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 |\uparrow\uparrow\rangle &= \frac{1}{2} (1(1+1)\hbar^2 - \frac{1}{2}(\frac{1}{2}+1)\hbar^2 - \frac{1}{2}(\frac{1}{2}+1)\hbar^2) |S = 1, M_S = 1\rangle \\
&= \frac{\hbar^2}{2} (2 - \frac{3}{4} - \frac{3}{4}) |S = 1, M_S = 1\rangle \\
&= \frac{\hbar^2}{4} |\uparrow\uparrow\rangle.
\end{aligned}$$

Hence $|\uparrow\uparrow\rangle$ is an eigenfunction of $\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2$ with eigenvalue $\hbar^2/4$.

Comment The identity given in the question follows because

$$\begin{aligned}\hat{\mathbf{S}}^2 &= \hat{\mathbf{S}} \cdot \hat{\mathbf{S}} \\ &= (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2) \cdot (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2) \\ &= \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_2 \\ &= \hat{\mathbf{S}}_1^2 + \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2^2 \\ &= \hat{\mathbf{S}}_1^2 + 2\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_2^2.\end{aligned}$$

In the last step we have used the fact that $\hat{\mathbf{S}}_1$ commutes with $\hat{\mathbf{S}}_2$. This is because $\hat{\mathbf{S}}_1$ acts only on spin kets referring to particle 1, while $\hat{\mathbf{S}}_2$ acts only on spin kets referring to particle 2, so the order of these operators does not matter.

Solution 6.4 We have

$$\begin{aligned}\langle S=1, M_S=0 | S=1, M_S=0 \rangle &= \frac{1}{2} (\langle \uparrow\downarrow | + \langle \downarrow\uparrow |) (\langle \uparrow\downarrow | + \langle \downarrow\uparrow |) \\ &= \frac{1}{2} (\langle \uparrow\downarrow | \uparrow\downarrow \rangle + \langle \uparrow\downarrow | \downarrow\uparrow \rangle + \langle \downarrow\uparrow | \uparrow\downarrow \rangle + \langle \downarrow\uparrow | \downarrow\uparrow \rangle).\end{aligned}$$

Now,

$$\begin{aligned}\langle \uparrow\downarrow | \uparrow\downarrow \rangle &= \langle \uparrow | \uparrow \rangle_1 \langle \downarrow | \downarrow \rangle_2 = 1 \times 1 = 1 \\ \langle \uparrow\downarrow | \downarrow\uparrow \rangle &= \langle \uparrow | \downarrow \rangle_1 \langle \downarrow | \uparrow \rangle_2 = 0 \times 0 = 0 \\ \langle \downarrow\uparrow | \uparrow\downarrow \rangle &= \langle \downarrow | \uparrow \rangle_1 \langle \uparrow | \downarrow \rangle_2 = 0 \times 0 = 0 \\ \langle \downarrow\uparrow | \downarrow\uparrow \rangle &= \langle \downarrow | \downarrow \rangle_1 \langle \uparrow | \uparrow \rangle_2 = 1 \times 1 = 1,\end{aligned}$$

so

$$\langle S=1, M_S=0 | S=1, M_S=0 \rangle = \frac{1}{2} (1 + 0 + 0 + 1) = 1.$$

Comment A two-particle inner product such as $\langle \uparrow\downarrow | \uparrow\downarrow \rangle$ uses the positional convention: the first entry in each bra or ket refers to particle 1, while the second entry refers to particle 2. This allows us to expand $\langle \uparrow\downarrow | \uparrow\downarrow \rangle$ as the product of $\langle \uparrow | \uparrow \rangle$ for particle 1 and $\langle \downarrow | \downarrow \rangle$ for particle 2. Both the single-particle inner products are easy to evaluate.

Solution 6.5 (a) The spatial function $\psi(x_1, x_2)$ is antisymmetric with respect to interchange of particle labels because

$$\begin{aligned}\psi(x_2, x_1) &= \frac{1}{\sqrt{2}} (\phi_A(x_2)\phi_B(x_1) - \phi_B(x_2)\phi_A(x_1)) \\ &= -\frac{1}{\sqrt{2}} (\phi_B(x_2)\phi_A(x_1) - \phi_A(x_2)\phi_B(x_1)) \\ &= -\frac{1}{\sqrt{2}} (\phi_A(x_1)\phi_B(x_2) - \phi_B(x_1)\phi_A(x_2)) \\ &= -\psi(x_1, x_2).\end{aligned}$$

(b) No. For spinless particles, the given spatial function would give an antisymmetric total wave function. This is inconsistent with the fact that spinless particles are bosons, and so must be described by a symmetric total wave function.

(c) Spin- $\frac{1}{2}$ particles are fermions. The total wave function is antisymmetric for identical fermions, so the given

spatial function must be accompanied by a symmetric spin ket. There are three possibilities:

$$|S = 1, M_S = 1\rangle = |\uparrow\uparrow\rangle$$

$$|S = 1, M_S = 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$|S = 1, M_S = -1\rangle = |\downarrow\downarrow\rangle,$$

all of which have $S = 1$, so we conclude that $S = 1$ in this case.

Comment To show that a given function $f(x_1, x_2)$ is antisymmetric under exchange of particle labels, write down an explicit function for $f(x_2, x_1)$ (with the labels reversed) and rearrange it to try to show that it is equal to $-f(x_1, x_2)$.

Solution 6.6 (a) A composite particle is a fermion if it contains an odd number of fermions; otherwise it is a boson. All spin- $\frac{1}{2}$ particles are fermions, including electrons, protons and neutrons. Hence:

1. A ${}^4\text{He}$ nucleus contains 4 fermions and is a boson.
2. A ${}^4\text{He}$ atom contains 6 fermions and is a boson.
3. A ${}^3\text{He}$ nucleus contains 3 fermions and is a fermion.
4. A ${}^3\text{He}$ atom contains 5 fermions and is a fermion.

(b) Because they are fermions, ${}^3\text{He}$ atoms do not normally undergo Bose–Einstein condensation. However, if pairs of ${}^3\text{He}$ can join together, each pair is a boson, and these pairs can undergo Bose–Einstein condensation at sufficiently low temperatures and sufficiently high number densities.

Comment At the number density found in the liquid phase, ${}^3\text{He}$ atoms combine together to form bosons at a few millikelvin above the absolute zero of temperature. At lower number densities, even lower temperatures are required.

Topic 7 — Measurement

Solution 7.1 (a) Immediately after the energy measurement, the system is in the eigenstate corresponding to the eigenvalue E_2 . The wave function is $\psi_2(x)e^{-iE_2 t/\hbar}$, multiplied by an arbitrary phase factor. The second energy measurement is certain to give the value E_2 .

(b) The system is in the stationary state $\psi_2(x)e^{-iE_2 t/\hbar}$, and remains in this state so long as it is not disturbed, so even after a considerable delay, the value E_2 is certain to be obtained.

(c) The position measurement results in a wave packet that is localized around the value of position that was obtained in the measurement. In general, this wave packet will be a linear superposition of many different energy eigenfunctions, not just those in the initial wave function. So, in this case, the second energy measurement could yield any of a wide range of values, and all we can say is that the result will be one of the energy eigenvalues of the system.

Comment As a general rule, when the resolution of the position measurement narrows, the spread of the energy values associated with the energy eigenfunctions widens. If the energy of the system is measured after a very precise position measurement, a value may be obtained that is very far from the initial energy. This can be reconciled with the general principle of energy conservation as the act of making a position measurement involves interaction with external apparatus and this can add or subtract energy from the quantum system under study.

Solution 7.2 Immediately after the spin component has been measured in the \mathbf{n} -direction, and the value $-\hbar/2$ has been obtained, the spin state of the particle is spin-down in the \mathbf{n} -direction. This is the same as being spin-up in the *minus* \mathbf{n} -direction. If the spin component is now measured in the z -direction, the probability that a value $+\hbar/2$ will be obtained is $\cos^2(\theta/2)$ where θ is the angle between the $-\mathbf{n}$ and $+z$ -directions. This angle is $\theta = 120^\circ$, so the required probability is

$$\text{probability} = \cos^2(120^\circ/2) = \cos^2 60^\circ = \left(\frac{1}{2}\right)^2 = \frac{1}{4}.$$

Comment The fact that the particle was initially prepared in a spin state with $S_z = +\hbar/2$ is irrelevant for the final spin measurement. This is because the spin measurement in the \mathbf{n} -direction causes the spin state vector to collapse, so all memory of the initial spin state is lost.

Topic 8 — Entanglement

Solution 8.1 The state $|\text{photon pair}\rangle$ is entangled because it cannot be represented as the product of a ket describing the state of photon 1, and another ket describing the state of photon 2. When the polarizations of both photons are measured relative to the z -axis, both photons give the same result. There is a 50% chance that the measurement will produce collapse onto $|\text{VV}\rangle$, with both photons vertically polarized, and there is a 50% chance that it will produce collapse onto $|\text{HH}\rangle$, with both photons horizontally polarized.

These correlations *can* be reproduced by a classical model in which pairs of photons are emitted at random in one of two ways: In 50% of cases both photons definitely have vertical polarization relative to the z -axis, and in the other 50% of cases both photons definitely have horizontal polarization relative to the z -axis.

Comment The predictions of quantum mechanics can be reproduced by a classical model *provided that* the polarization measurements all refer to measurements along the z -axis. Furthermore, in quantum mechanics the state $|\text{photon pair}\rangle$ produces perfect correlations (in which measurements on the two photons agree) no matter which single axis is chosen for the measurements. Even this can be accounted for by a more elaborate classical model. However, partial correlations still persist when the two polarization measurements use different axes. For example, there is a high probability of agreement when the two observers use axes that point in almost the same direction, and there is a low probability of agreement when they use axes that differ by almost 90° . When a range of different axis pairs is used, and precise probabilities calculated, classical physics is unable to reproduce all predictions of quantum mechanics.

Solution 8.2 We have

$$\begin{aligned}\langle A|A\rangle &= \frac{1}{3} [(\langle \uparrow_x \uparrow_y | + \langle \uparrow_y \uparrow_x |)(|\uparrow_x \uparrow_y\rangle + |\uparrow_y \uparrow_x\rangle)] \\ &= \frac{1}{3} [\langle \uparrow_x \uparrow_y | \uparrow_x \uparrow_y\rangle + \langle \uparrow_x \uparrow_y | \uparrow_y \uparrow_x\rangle + \langle \uparrow_y \uparrow_x | \uparrow_x \uparrow_y\rangle + \langle \uparrow_y \uparrow_x | \uparrow_y \uparrow_x\rangle].\end{aligned}$$

Now

$$\langle \uparrow_x | \uparrow_x \rangle = 1$$

$$\langle \uparrow_y | \uparrow_y \rangle = 1$$

$$\langle \uparrow_x | \uparrow_y \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} = \frac{1}{2}(1+i)$$

$$\langle \uparrow_y | \uparrow_x \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -i \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{2}(1-i),$$

so we have

$$\langle \uparrow_x \uparrow_y | \uparrow_x \uparrow_y \rangle = \langle \uparrow_x | \uparrow_x \rangle \langle \uparrow_y | \uparrow_y \rangle = 1 \times 1 = 1$$

$$\langle \uparrow_x \uparrow_y | \uparrow_y \uparrow_x \rangle = \langle \uparrow_x | \uparrow_y \rangle \langle \uparrow_y | \uparrow_x \rangle = \frac{1}{2}(1+i) \times \frac{1}{2}(1-i) = \frac{1}{2}$$

$$\langle \uparrow_y \uparrow_x | \uparrow_x \uparrow_y \rangle = \langle \uparrow_y | \uparrow_x \rangle \langle \uparrow_x | \uparrow_y \rangle = \frac{1}{2}(1-i) \times \frac{1}{2}(1+i) = \frac{1}{2}$$

$$\langle \uparrow_y \uparrow_x | \uparrow_y \uparrow_x \rangle = \langle \uparrow_y | \uparrow_y \rangle \langle \uparrow_x | \uparrow_x \rangle = 1 \times 1 = 1.$$

Consequently,

$$\langle A|A\rangle = \frac{1}{3} \left[1 + \frac{1}{2} + \frac{1}{2} + 1 \right] = 1.$$

The probability *amplitude* for both particles to be measured to be spin-up in the x -direction is

$$\begin{aligned}
\langle \uparrow_x \uparrow_x | A \rangle &= \frac{1}{\sqrt{3}} [\langle \uparrow_x \uparrow_x | \uparrow_x \uparrow_y \rangle + \langle \uparrow_x \uparrow_x | \uparrow_y \uparrow_x \rangle] \\
&= \frac{1}{\sqrt{3}} [\langle \uparrow_x | \uparrow_x \rangle \langle \uparrow_x | \uparrow_y \rangle + \langle \uparrow_x | \uparrow_y \rangle \langle \uparrow_x | \uparrow_x \rangle] \\
&= \frac{1}{\sqrt{3}} \left[1 \times \frac{1}{2}(1+i) + \frac{1}{2}(1+i) \times 1 \right] \\
&= \frac{1}{\sqrt{3}} (1+i).
\end{aligned}$$

The corresponding probability is

$$\text{probability} = |\langle \uparrow_x \uparrow_x | A \rangle|^2 = \frac{1}{3}(1+i)(1-i) = \frac{2}{3}.$$

Comments (1) In this case the normalization constant is $1/\sqrt{3}$ rather than $1/\sqrt{2}$. This is because $|\uparrow_x\rangle$ is not orthogonal to $|\uparrow_y\rangle$ (see Exercise 5.1).

(2) The probability of any pair of spin measurements in a two-particle spin state $|A\rangle$ can be calculated in a similar way. The probability that particle 1 has spin a and particle 2 has spin b is $|\langle ab|A\rangle|^2$.

Topic 9 — Polarization states of photons

Solution 9.1 (a) We have $\langle V|V\rangle = \langle H|H\rangle = 1$ and $\langle V|H\rangle = \langle H|V\rangle = 0$. So

$$\begin{aligned}
\langle V_\theta | V_\theta \rangle &= (\cos \theta \langle V | + \sin \theta \langle H |) (\cos \theta | V \rangle + \sin \theta | H \rangle) \\
&= \cos^2 \theta \langle V | V \rangle + \cos \theta \sin \theta \langle V | H \rangle + \sin \theta \cos \theta \langle H | V \rangle + \sin^2 \theta \langle H | H \rangle \\
&= \cos^2 \theta + \sin^2 \theta = 1.
\end{aligned}$$

$$\begin{aligned}
\langle H_\theta | H_\theta \rangle &= (-\sin \theta \langle V | + \cos \theta \langle H |) (-\sin \theta | V \rangle + \cos \theta | H \rangle) \\
&= \sin^2 \theta \langle V | V \rangle - \sin \theta \cos \theta \langle V | H \rangle - \cos \theta \sin \theta \langle H | V \rangle + \cos^2 \theta \langle H | H \rangle \\
&= \sin^2 \theta + \cos^2 \theta = 1.
\end{aligned}$$

$$\begin{aligned}
\langle H_\theta | V_\theta \rangle &= (-\sin \theta \langle V | + \cos \theta \langle H |) (\cos \theta | V \rangle + \sin \theta | H \rangle) \\
&= -\sin \theta \cos \theta \langle V | V \rangle - \sin^2 \theta \langle V | H \rangle + \cos^2 \theta \langle H | V \rangle + \cos \theta \sin \theta \langle H | H \rangle \\
&= -\sin \theta \cos \theta + \cos \theta \sin \theta = 0.
\end{aligned}$$

There is need to calculate $\langle V_\theta | H_\theta \rangle$ because we always have $\langle V_\theta | H_\theta \rangle = \langle H_\theta | V_\theta \rangle^*$.

(b) The equations for photons involve θ rather than $\theta/2$.

Comment The states $|V_\theta\rangle$ and $|H_\theta\rangle$ represent vertical and horizontal polarizations relative to an axis that is rotated by an angle θ from the axis chosen to define V and H . The sense of rotation matters because, for example, $|V_{30}\rangle$ is not the same as $|V_{-30}\rangle$. We adopt the following convention: if the photon travels in the y -direction, and the z -direction is associated with V , the positive sense of rotation is from the z -direction towards the x -direction.

Solution 9.2 The probability amplitude for right-handed circular polarization is

$$\begin{aligned}\langle \mathbf{R}|A\rangle &= -\frac{1}{\sqrt{2}}(\langle \mathbf{H}| - i\langle \mathbf{V}|)(a_1|\mathbf{H}\rangle + a_2|\mathbf{V}\rangle) \\ &= -\frac{1}{\sqrt{2}}(a_1\langle \mathbf{H}|\mathbf{H}\rangle - ia_1\langle \mathbf{V}|\mathbf{H}\rangle + a_2\langle \mathbf{H}|\mathbf{V}\rangle - ia_2\langle \mathbf{V}|\mathbf{V}\rangle).\end{aligned}$$

The linear polarization states $|\mathbf{H}\rangle$ and $|\mathbf{V}\rangle$ are orthonormal, so $\langle \mathbf{H}|\mathbf{H}\rangle = \langle \mathbf{V}|\mathbf{V}\rangle = 1$ and $\langle \mathbf{H}|\mathbf{V}\rangle = \langle \mathbf{V}|\mathbf{H}\rangle = 0$. Hence,

$$\langle \mathbf{R}|A\rangle = -\frac{1}{\sqrt{2}}(a_1 - ia_2).$$

The corresponding probability for right-handed circular polarization is

$$\begin{aligned}|\langle \mathbf{R}|A\rangle|^2 &= \left| -\frac{1}{\sqrt{2}}(a_1 - ia_2) \right|^2 \\ &= \frac{1}{2}(a_1 - ia_2)(a_1 + ia_2) \\ &= \frac{1}{2}(a_1^2 + a_2^2) \\ &= \frac{1}{2},\end{aligned}$$

because a_1 and a_2 are real and $a_1^2 + a_2^2 = 1$.

Comment Any state of polarization can be written as a linear combination of $|\mathbf{H}\rangle$ and $|\mathbf{V}\rangle$:

$$|\text{polarization state}\rangle = c_1|\mathbf{H}\rangle + c_2|\mathbf{V}\rangle,$$

where $|c_1|^2 + |c_2|^2 = 1$.

If c_2/c_1 is a real number, or if $c_1 = 0$, the state describes linear polarization. If c_2/c_1 is an imaginary number, the state describes circular polarization. When c_2/c_1 is neither real nor imaginary, the states are neither linearly polarized nor circularly polarized. (These states are said to correspond to elliptical polarization, but they are not discussed in this course.)

Solution 9.3 We have

$$\begin{aligned}|\mathbf{R}_\theta\rangle &= -\frac{1}{\sqrt{2}}[|\mathbf{H}_\theta\rangle + i|\mathbf{V}_\theta\rangle] \\ &= -\frac{1}{\sqrt{2}}[(-\sin\theta|\mathbf{V}\rangle + \cos\theta|\mathbf{H}\rangle) + i(\cos\theta|\mathbf{V}\rangle + \sin\theta|\mathbf{H}\rangle)].\end{aligned}$$

Collecting together terms,

$$\begin{aligned}|\mathbf{R}_\theta\rangle &= -\frac{1}{\sqrt{2}}[(\cos\theta + i\sin\theta)|\mathbf{H}\rangle + (-\sin\theta + i\cos\theta)|\mathbf{V}\rangle] \\ &= -\frac{1}{\sqrt{2}}[(\cos\theta + i\sin\theta)|\mathbf{H}\rangle + i(\cos\theta + i\sin\theta)|\mathbf{V}\rangle],\end{aligned}$$

and Euler's formula gives

$$|\mathbf{R}_\theta\rangle = -\frac{1}{\sqrt{2}}e^{i\theta}(|\mathbf{H}\rangle + i|\mathbf{V}\rangle) = e^{i\theta}|\mathbf{R}\rangle.$$

Similarly,

$$\begin{aligned}|\mathbf{L}_\theta\rangle &= \frac{1}{\sqrt{2}}[|\mathbf{H}_\theta\rangle - i|\mathbf{V}_\theta\rangle] \\ &= \frac{1}{\sqrt{2}}[(-\sin\theta|\mathbf{V}\rangle + \cos\theta|\mathbf{H}\rangle) - i(\cos\theta|\mathbf{V}\rangle + \sin\theta|\mathbf{H}\rangle)].\end{aligned}$$

Collecting together terms,

$$\begin{aligned} |L_\theta\rangle &= \frac{1}{\sqrt{2}} [(\cos \theta - i \sin \theta)|H\rangle + (-\sin \theta - i \cos \theta)|V\rangle] \\ &= \frac{1}{\sqrt{2}} [(\cos \theta - i \sin \theta)|H\rangle - i(\cos \theta - i \sin \theta)|V\rangle], \end{aligned}$$

and Euler's formula gives

$$|L_\theta\rangle = \frac{1}{\sqrt{2}} e^{-i\theta} (|H\rangle - i|V\rangle) = e^{-i\theta} |L\rangle.$$

These calculations show that $|R_\theta\rangle$ differs from $|R\rangle$ only by a multiplicative phase factor $e^{i\theta}$, and $|L_\theta\rangle$ differs from $|L\rangle$ only by a multiplicative phase factor $e^{-i\theta}$. Such phase factors are unimportant and do not change the physical states being described.

Comment The ket vectors $|V_\theta\rangle$ and $|H_\theta\rangle$ describe states of vertical and horizontal polarization relative to an axis that is rotated by an angle θ from the axis used to define V and H . However, we have the freedom to choose axes however we wish, so there should be no physical distinction between $|R\rangle$ and $|R_\theta\rangle$. This is confirmed by the above explicit calculation.

Solution 9.4 Using

$$|R\rangle = -\frac{1}{\sqrt{2}} (|H\rangle + i|V\rangle) \quad \text{and} \quad |L\rangle = \frac{1}{\sqrt{2}} (|H\rangle - i|V\rangle),$$

we obtain

$$\begin{aligned} |LR\rangle &= -\frac{1}{2} (|H\rangle - i|V\rangle)_1 (|H\rangle + i|V\rangle)_2 \\ &= -\frac{1}{2} (|H\rangle_1|H\rangle_2 + i|H\rangle_1|V\rangle_2 - i|V\rangle_1|H\rangle_2 + |V\rangle_1|V\rangle_2) \\ &\equiv -\frac{1}{2} (|HH\rangle + i|HV\rangle - i|VH\rangle + |VV\rangle). \end{aligned}$$

Similarly,

$$\begin{aligned} |RL\rangle &= -\frac{1}{2} (|H\rangle + i|V\rangle)_1 (|H\rangle - i|V\rangle)_2 \\ &= -\frac{1}{2} (|H\rangle_1|H\rangle_2 - i|H\rangle_1|V\rangle_2 + i|V\rangle_1|H\rangle_2 + |V\rangle_1|V\rangle_2) \\ &\equiv -\frac{1}{2} (|HH\rangle - i|HV\rangle + i|VH\rangle + |VV\rangle). \end{aligned}$$

Subtracting these two results and multiplying by $1/\sqrt{2}$ then gives

$$|A\rangle = \frac{1}{\sqrt{2}} (|LR\rangle - |RL\rangle) = \frac{i}{\sqrt{2}} (|VH\rangle - |HV\rangle),$$

as required.

If photon 1 is measured with left-handed circular polarization (L), then the state vector collapses onto the first term on the left-hand side, and photon 2 is certain to be measured with right-handed circular polarization (R). Similarly, if photon 1 is measured with right-handed circular (R) polarization, the state vector collapses onto the second term on the left-hand side, and photon 2 is certain to be measured with left-handed circular polarization (L). So the two observers always disagree about the circular polarizations of the two photons.

A similar argument shows that, if photon 1 is measured with horizontal linear polarization (H), then photon 2 is certain to be measured with vertical linear polarization (V), and if photon 1 is measured with vertical linear polarization (V), then photon 2 is certain to be measured with horizontal linear polarization (H). So the two observers always disagree about the linear polarizations of the two photons relative to the z -axis.

Comment The usual formulas used to convert $|H\rangle$ and $|V\rangle$ into $|R\rangle$ and $|L\rangle$ assume that the directions associated with H and V (in that order) are related to the direction of motion of the photon by the right-hand rule. If both

photons travel in the same direction, this assumption can be valid for both photons and we can use the same conversion formula throughout. This is what we have done in answering this question. However, the same assumption would not be valid for photons travelling in opposite directions, as occurs in a typical Aspect experiment. You are not expected to remember this detail, which is included only for completeness.

Topic 10 — Quantum information

Solution 10.1 (a) Two bases are complementary if any state that is certain to produce a given value of the observable in one basis has equal probabilities of producing the two alternative values in the other basis.

- (b) 45°
- (c) 90° .

Comment As usual, the result for the spin of a spin- $\frac{1}{2}$ particle involves half the angle of the result for the polarization of a photon.

Solution 10.2 (a) It is essential for Alice and Bob to use the same basis, so cases 1, 3, 7 and 8 can be rejected.

(b) In cases 5 and 9, Alice and Bob use the same basis, but get different results. These cases suggest that an eavesdropper might be present.

Comment In practice, noisy transmission channels for the photons and inefficient detection equipment can lead to a small error rate when Bob and Alice use the same basis in the absence of an eavesdropper. In real applications, the non-eavesdropper error rate is estimated and eavesdropping declared only when the measured error rate exceeds this estimate.

Solution 10.3 (a) The two measurements in which Alice and Bob measure polarization in the same direction (both 22.5° or both 45°) are used directly to prepare a cryptographic key. For the given entangled state, Alice's measurements are anti-correlated with Bob's — if Bob measures vertical polarization, Alice measures horizontal polarization and vice versa. If Bob converts vertical polarization to the digit 1, and horizontal polarization to the digit 0, Alice must use the opposite convention, converting horizontal polarization to 1, and vertical polarization to 0. Then they both have the same random cryptographic key.

(b) The remaining measurements are used to verify that eavesdropping has not taken place. On the basis of many results, Bob and Alice compute

$$\Sigma = C(\alpha_1 - \beta_1) + C(\alpha_1 - \beta_2) + C(\alpha_2 - \beta_1) - C(\alpha_2 - \beta_2)$$

where $C(\alpha_i - \beta_j)$ is a correlation function giving the proportion of times Bob and Alice agree minus the proportion of times they disagree about their polarization measurements on a photon pair when Alice uses angle α_i and Bob uses angle β_j . In this expression, α_1 and α_2 are Alice's angles (0 and 45°) and β_1 and β_2 are Bob's angles (22.5° and -22.5°). Using the formula for the correlation function given in the question, we obtain

$$\begin{aligned} \Sigma &= -\cos[2(0^\circ - 22.5^\circ)] - \cos[2(0^\circ + 22.5^\circ)] - \cos[2(45^\circ - 22.5^\circ)] + \cos[2(45^\circ + 22.5^\circ)] \\ &= -\cos(-45^\circ) - \cos(45^\circ) - \cos(45^\circ) + \cos(135^\circ) \\ &= -2\sqrt{2}. \end{aligned}$$

A result like this (with a magnitude greater than 2) is only possible because the photons are entangled and have non-local correlations. If eavesdropping takes place, the photons cease to be entangled and Σ must then satisfy the Bell inequality $|\Sigma| \leq 2$. Hence, eavesdropping is guarded against by checking that $|\Sigma|$ is much closer to $2\sqrt{2}$ than 2.

Comment With the angles $\alpha_1, \alpha_2, \beta_1$ and β_2 chosen in the question, $|\Sigma| > 2$, in violation of Bell's inequality. But if we labelled these angles in a different way, say with β_1 and β_2 interchanged, we would find no such violation. This is not a problem. The fact that some ways of labelling the angles do not challenge Bell's inequality does not affect our conclusion; the only thing that matters is that there is a way of labelling the angles that violates the inequality. To challenge Bell's inequality as strongly as possible, it is important that the last term in the CHSH sum (the one prefaced with a minus sign) should refer to a large angle and the other three terms (prefaced with plus signs) should refer to smaller angles.

Solution 10.4 Because the Bell-state measurement gives a result corresponding to $|\Psi^+\rangle_{12}$, the three-photon state $|\Psi\rangle_{123}$ collapses onto $|\Psi^+\rangle_{12}|B\rangle_3$. So, after the measurement, photon 3 is in the state

$$|B\rangle = \begin{bmatrix} -\alpha \\ \beta \end{bmatrix}.$$

This is not quite the same as the initial state of photon 1, but it is closely related to it. If the person (Alice) who conducted the Bell-state measurement opens up a classical communication channel and talks to a person (Bob) who is able to adjust the state of photon 3, the news that the Bell-state measurement on photons 1 and 2 gave a result corresponding to $|\Psi^+\rangle_{12}$ is sufficient to tell Bob to reverse the first component of the state vector for photon 3 and leave the other component unchanged. Equivalently, Bob can apply the linear transformation

$$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -\alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}.$$

Once this is done, the polarization state of photon 3 is the same as the initial (unknown) polarization state of photon 1.

The no-cloning theorem is not violated because, after the Bell-state measurement, photon 1 is no longer in its initial state, and all trace of this state is lost in the Bell state $|\Psi^+\rangle_{12}$ that exists after the measurement.

Comment The teleportation described in this question has been achieved in real experiments.